A thesis
on the
spatial localization of
the harmonic oscillator
by
K. D. Wiens
in partial fulfillment
of the requirements for
the Master of Science Degree
from the
University of Manitoba

PREFACE

This thesis is part of a series in a study leading to the incorporation of localization theory in the analysis of low energy collisions between atomic and molecular species. The material presented here has been extended to the hydrogen atom so that a proton-hydrogen atom system can be studied. Dr. R. Wallace is gratefully thanked for his stimulating ideas and guidance in directing the work of this thesis.

ABSTRACT

Various methods of localization are defined in order to create a set of local states for a one-dimensional harmonic oscillator. The mean parameters of these states are evaluated and some discussion is given to the possible problems associated with each method in extending the calculations to the hydrogen atom. The fundamental properties of a local representation are derived and their application to a general collision problem is considered.

CONTENTS

TABLES

FIGURES

LIST OF SYMBOLS EMPLOYED IN THE THESIS

Ψ	DENOTES A LOCAL STATE
ψ	DENOTES A NON-LOCAL STATE
a, b	BOUNDARY LIMITS
$S(x-x_o)$	STEP FUNCTION
$\theta(a,b)$	HEAVISIDE FUNCTION
$\delta(x)$	DIRAC DELTA FUNCTION
δ_{kn}	KRONECKER-DELTA SYMBOL
$\langle\ \rangle$	DENOTES A MEAN VALUE
H	HAMILTONIAN
E	ENERGY
L	FINITE DIFFERENCE OPERATOR
α	PARAMETER CONTROLLING THE HERMITIAN NATURE OF AN OPERATOR
Δ	DENOTES UNCERTAINTY
x	POSITION VECTOR
p	MOMENTUM VECTOR
N	NORMALIZATION CONSTANT
$H_n(x)$	N^{TH} HERMITE POLYNOMIAL
$(1-\delta_{kn})$	DENOTES ONLY OFF DIAGONAL TERMS OF A MATRIX

INTRODUCTION

This thesis originated in considering atomic and molecular collisions, and in particular, a hydrogen-proton low energy process. Collision theory calculations are usually performed with some approximation such as the Born series approach (1) for high energy collisions or the distorted wave method (2) for lower energy or molecular rearrangement processes. A conceptual difficulty arises in using the Schrodinger wave equation approach as the eigenfunctions of atoms and molecules are non-local (i.e. they are formulated using an infinite domain.). One can not talk of an isolated system before or after a collision, but only of an infinitely continuous, reacting domain. This formulation, which uses an infinite domain, leads to practical difficulties in obtaining suitable wave functions with correct boundary conditions (2). These problems are usually avoided by neglecting coupling terms and/or overlap integrals at large separations. This difficulty becomes more noticeable for atoms with many electrons as a one-electron approach is used for solving these systems. Although the electron cloud becomes more diffuse in space it is still meaningful for an experimentalist to speak of the electron as located in a finite region of space and time.

The concept of causality has always been a conceptually weak point of quantum mechanics. The Copenhagen interpretation, symbolically stated by $\Delta x \Delta p \leq \Delta E \Delta t \leq \hbar$, emphasizes the uncontrollable influence of the measurement procedure. Consequently, the wave function has come to represent the probability of possible results of a measurement; that is, it represents our knowledge of events and not the behaviour of the electron. This lack of causality then prevents a detailed look at the mechanism of a collision reaction.

A search for a more physical interpretation of quantum mechanics has been present since this formalism was accepted at the Fifth Solvay Conference.

J. Von Neumann (3) mathematically formalized quantum mechanics and asserted that: " The present system of quantum mechanics would have to be objectively false, in order that another description of the elementary processes than the statistical one be possible." Consequently he viewed quantum theory as being complete. Einstein, Podolsky, and Rosen (4) defined completeness by: " Every element of physical reality must have a counterpart in the physical theory." and they created a wave function that yielded two elements of reality. This is the famous Einstein, Podolsky, Rosen paradox which has prompted much of the present day research, especially hidden variable theory (5,6,7,8), on the interpretation of the wave function.

D. Bohm and J. Bub (9) developed a hidden variable theory to add causality to a process that is similar to the above collision problem, and it is known as the measurement process. If an operator R with eigenvalue R_i operates on a wave function $\Psi(x) = \sum \psi_i R_i(x)$ it yields R_i. This process is known as reduction of a wave packet and it is important as it ensures reproducibility of results. Bohm and Bub use an extension of Siegl and Wiener's ideas (10) and couple the measuring apparatus to the observed system. A non-linear and a very non-local, irreversible equation of motion is developed. Instrumentation to record the phenomena and times involved with this theory has not yet been developed and J. H. Tutsch (11) has investigated whether the times are theoretically measureable. His collapse time, (11) although extremely short, did

did not violate the uncertainty principle and therefore is technically measureable. Other work on this problem has been done by Daneri, Loinger, and Prosperi (12).

The quantum theory of measurement is also investigated by A. L. Licht (13) by considering the local character of the process of measurement and the preparation of the state. The local state is constructed by examining a bounded interval set up by a finite observer and some infinite region or background which the experimenter can not completely know or control. A set of states can accordingly be generated whose local character can be affected by past events in the background state, or be independent of them, or have some composite type of locality.

Hidden variable theory has lead to research on stochastic theory influencing quantum mechanics. Bohm and Vigier (14) sugested that the uncertainty relation could be caused by random fluctations arising from a subquantum medium (5). Various authors (15,16,17) have used this to derive the Schrodinger equation with generalized mechanics (16,17) and thus avoided the ambiguous concept of the correspondence rule (18). One of the most interesting features of the theory is that the wave function is no longer considered a complete description of the state (16). Hidden variable theory is a natural part of this (17), and the measurement problem is partially explained in that the limit of the precision of measurement is also a feature of macroscopic brownian motion. This work has reconverted L.De Broglie (19,20) to a causal approach in the interpretation of the wave function. He has localized the electron using wave mechanics by treating the electron as being subjected to a brownian motion caused by the subquantum potential.

The collision problem can be resolved if one defines a local state. This would then remove the asymptotic problems associated with a diffuse wave function and a molecular species would remain isolated until its domain overlapped another. Such a proposal would naturally provide a mechanism for threshold radii and energy. The axiom of distant systems being independent of each other is present in literature (6,18) and considerable emphasis is now being placed on localizability, and its integration into the framework of quantum mechanics. This thesis is directed along this problem and investigates the methods and characteristics of a system as its domain is varied finitely.

Much of the work on localizability has originated from elementary particle physics. W. Pauli (21), in 1932, realized that the photon was non-local, mathematically, and yet experimentally it appears as a sharp signal . T.D. Neuton and E.P. Wigner (23) succeeded in creating a local state for particles of non-zero mass and arbitrary spin.The localizing functions belong to the position operator set which preserves the positive energy character of a wave function. Their work was mathematically formulated into quantum mechanics by A.S. Wightman (24).

" The notion of localizability comprises two different aspects, one which expresses the fact that there exist a family of observables each of which corresponds to the question whether the system is contained within a certain region in space, and another which expresses the homogeneity and isotropy of space (25) ". Jauch and Piron (25) generalize localizability by omitting the postulate that all observations of position measurements are compatible with one another. They also introduce the concept of weakly and nearly localizable systems by weakening their initial hypothesis. This is similar to A.L. Licht's states which can vary in their local nature. It is the former aspect of localizability that Schrodinger overlooked in his initial papers on quantum mechanics as the calculations are so numerous that they can only be solved by a computer.

The concept of an infinite domain is one of the basic postulates of quantum mechanics. E.Schrodinger assumed that it was over the "whole co-ordinate space (26) ", but further clarified his viewpoint with the statement " this formulation is not entirely ambiguous (26) ". In considering the hydrogen atom, Schrodinger developed a differential equation with singularities at zero and infinity. These, in his opinion, form the "bounding points of our real interval (27) " and the " postulation of the finiteness of the wave function at the bounding points is equivalent to a boundary condition. (27) " At first Schrodinger thought that the lack of knowledge of the boundary condition would give him too extensive a manifold of solutions but finally concluded that " the equation carries within itself the quantum conditions (28) " and " the quantum levels are at once defined as the proper values of the equation, which carries in itself its natural boundary conditions (29). " These boundary conditions were those that gave a correct energy spectrum. In all other work both Schrodinger and Heisenberg refer to the domain as the " natural boundary value problem (30). " Obviously for an infinite domain a zero endpoint uniquely defines the quantum condition. However, as the domain becomes finite a zero endpoint for the wave function can still define a set of quantum conditions that can yield experimental results. These results were never proven to be wrong solutions by Schrodinger. His approach represented a reversal in thought from the classical viewpoint of a domain, and the early quantum mechanical one which had localization as a fundamental feature (31). It is basically a minute electron density, past about 20 a.u.,which does not affect the mean parameters of the system, and which creates the Einstein, Podolsky, Rosen paradox and other conceptual problems.

CONSTRUCTION OF LOCAL STATES

Two different methods exist for constructing a local state, a bounded operator or Heisenberg approach, or a wave packet or Schrodinger approach. The wave packet method requires that the end-point be defined as zero past the bounded interval, while the operator method demands that a boundary condition is necessary to establish the hermitian nature.

The bounded operator method has already been suggested by J. Von Neumann (32). For the operator $-i\hbar d/dq$ in the interval of $a \leq q \leq b$ the differential equation is:

$$-i\hbar d/dq\ f(q) = \lambda f(q) \qquad 1$$

$$f(q) = ce^{2\pi i \lambda q/h} \qquad 2$$

The boundary condition is:

$$f(a):f(b) = e^{2\pi i \lambda (a-b)/h} = e^{-i\alpha} \qquad (0 \leq \alpha \leq 2\pi) \qquad 3$$

$$2\pi i \lambda (a-b)/h = -i\alpha - 2k\pi i \qquad k = 0, \pm 1, \pm 2 \qquad 3a$$

Using the normalization integral the wave function becomes:

$$\Psi(q) = \frac{1}{(a-b)^{\frac{1}{2}}} e^{2\pi i(\alpha/2\pi + k)q/(a-b)} \qquad 4$$

This constructs an orthonormal and complete set which gives a discrete spectrum. The boundary condition α , controls the hermitian nature of the operator and has a profound influence on the eigenvalues and eigenvectors. This process is essentially different for the infinite domain case (33), as equation 4 represents a series of plane waves which are unnormalizable on the infinite domain.

The other method of localization is via wave mechanics. In this approach the wave packet has as its " shaping function " or " envelope " a square wave which controls the domain of the wave function. As the square wave, numerically equal to one within the domain, is not a mathematical function in the normal sense (see appendix A), its end points must be defined by a Laurent series. If $\psi(x)$ represents a wave function satisfying the infinite boundary condition for the differential equation, then the local wave function will be described by:

$$\Psi(x) = N\psi(x)\theta(a,b) \tag{5}$$

$\theta(a,b)$ is called the Heaviside step function and governs the endpoints a and b. N is a normalization constant given as follows:

$$\langle\Psi|\Psi\rangle = \int_{-\infty}^{+\infty} \langle\Psi|x\rangle\langle x|\Psi\rangle\, dx \tag{6}$$

$$= N^2\int_{-\infty}^{+\infty} \psi^*(x)\theta(a,b)^2\psi(x)dx \tag{7}$$

$$N = \left\{\int_a^b \psi^*(x)\psi(x)dx\right\}^{-\frac{1}{2}} \tag{8}$$

Several properties of localization can readily be seen from the following derivation. First, the probability that a particle is localized in a region is given by:

$$P(a \leq x \leq b) = \int_a^b \psi^*(x)\psi(x)dx \tag{9}$$

The probability that the energy is the energy of the state is:

$$P(E = E_n) = \langle\Psi|\psi\rangle\langle\psi|\Psi\rangle \tag{10}$$

$$= |\langle\Psi|\psi\rangle|^2 \tag{11}$$

$$= \left\{N\int_{-\infty}^{+\infty} \psi^*(x)\theta(a,b)^2\psi(x)dx\right\}^2 \tag{12}$$

$$P(E=E_n)=\int_a^b \psi^*(x)\psi(x)dx \quad . \tag{13}$$

$$=P(a\leq x\leq b) \tag{14}$$

This derivation indicates that a local state is more general, with the transition from a classical to infinite domain being continuous. Furthermore, the concept of a stationary state, or a dispersion free state is overcome. Such a state has the property $\langle A\rangle^2 = \langle A^2\rangle$ for an observable. One of Von Neumann's (3) first conclusions in his classic theorem on completeness was to indicate that there is no physically meaningful density matrix which gives zero dispersion. In localization theory ΔE is not zero as it is with a stationary state, and it can be adjusted to within experimental error. This slight uncertainty in energy then allows the particle to be more localized in $\{x\}$ space. However because of the general properties of the fourier integral Δp increases while $\Delta x\Delta p\leq\frac{1}{2}h$ still is satisfied. This general feature removes the conceptual problems involving atomic collisions.

The mathematical model used is the one-dimensional harmonic oscillator. This provides a differential equation with no singularities and therefore it is a mathematically simple model. It suffers from the drawback that it is an idealization and can not be tested expermentally. However, the techniques involved can be generalized to a three dimensional real system, i.e. the hydrogen atom. The degree of localization is arbitrary and is dependent upon the system. In this thesis, localization will be expressed as a function of the domain up to and including the classical bound. Atomic units are used in all calculations. The various constants are removed in the following manner. For a harmonic oscillator of mass m and oscillating frequency ω, the hamiltonian is:

$$\mathcal{H}=\frac{1}{2m}\left(p^2+m^2\omega^2q^2\right) \qquad 15$$

Then define

$$\mathcal{H}=H\hbar\omega \qquad 16$$

$$q=(\hbar/m\omega)^{\frac{1}{2}}Q \qquad 17$$

$$p=(m\hbar\omega)^{\frac{1}{2}}P \qquad 18$$

$$H=\tfrac{1}{2}(P^2+Q^2) \qquad 19$$

The one dimensional Schrodinger equation is then:

$$\tfrac{1}{2}(-d^2/dq^2+q^2)\,\psi_n(q)=E_n\psi_n(q) \qquad 20$$

$$\psi_n(q)=(\sqrt{\pi}\,2^n n\,!)^{-\frac{1}{2}}\;e^{-\frac{1}{2}q^2}\;H_n(q) \qquad 21$$

$H_n(q)$ represents the n^{th} Hermite polynomial.

WAVE PACKET APPROACH

Initially, an attempt was made to construct a local wave function by taking a linear combination of eigenfunctions. The coefficients were then varied to give a zero overlap past a cut off radius. This failed because a singular set of points was generated, and consequently only an approximate set of coefficients were obtained. This gave a reduced electron density past the cut off radius.

To achieve a zero electron density beyond the domain it was necessary to change the envelope of the wave function by using the Heaviside step function (see appendix A), so that the wave packet is identically zero outside the bound. The endpoint then is defined in a generalized manner (via distribution theory (34,35)) by a Laurent series.

The localized function is given by equation 5. An assumption was made from step 7 to 8, namely $\theta^2(a,b) \equiv \theta(a,b)$. This can be seen intuitively. However, products of distributions are not necessarily defined unless there is support for each function in the domain. Then two generalized functions can be defined as being equivalent if they both have the same limit for the Laurent series describing the distributions. A more rigorous approach to this problem is given by M.J. Lighthill (35). Further problems will occur with the derivatives of distributions.

Using equation 5 the mean parameters of the system can be calculated using the usual set of algorithms.

$$\langle E \rangle = \tfrac{1}{2}\left\{\langle p^2 \rangle + \langle x^2 \rangle\right\} \qquad 22$$

$$\langle p^2 \rangle = \langle \Psi | p^2 | \Psi \rangle \qquad 23$$

$$\langle p^2\rangle = \int\int \langle \Psi|x'\rangle\, dx'\, \langle x'|p^2|x''\rangle\, dx''\, \langle x''|\Psi\rangle\, \delta(x'-x'')dx'dx'' \qquad 24$$

$$= -\int_{-\infty}^{+\infty} N\psi(x)\theta(a,b)\, \frac{d^2}{dx^2}\Big[N\psi(x)\theta(a,b)\Big]\, dx \qquad 25$$

$$= -N^2\int_{-\infty}^{+\infty} \theta(a,b)\theta(a,b)\psi^2(x)dx - 2N^2\int_{-\infty}^{+\infty} \psi'(x)\psi(x)\cdot \theta'(a,b)\theta(a,b)dx - N^2\int_{-\infty}^{+\infty} \psi''(x)\theta(a,b)^2\psi(x)dx \qquad 26$$

In the above derivation the wave functions are real. To evaluate the derivatives of the Heaviside step function it is necessary to use the following definition: If $\phi(x)$ is a distribution with m derivatives and f(x) is a continuous well behaved function vanishing outside some bounded domain, with m derivatives, then (35):

$$\int_{-\infty}^{+\infty} \phi^m(x)f(x)dx = (-1)^m\int_{-\infty}^{+\infty} \phi(x)f^m(x)dx \qquad 27$$

This formula can be derived by applying integration by parts m times. Using equation 27, the mean kinetic energy can be simplified to:

$$\langle p^2\rangle = -N^2\int_{-\infty}^{+\infty} \psi''(x)\theta(a,b)\psi(x)dx + N^2\int_{-\infty}^{+\infty} \theta'(a,b)^2\psi^2(x)dx \qquad 28$$

The mean potential energy is given by:

$$\langle x^2\rangle = N^2\int_{-\infty}^{+\infty} \psi^2(x)\theta(a,b)x^2dx \qquad 29$$

Using the Schrodinger equation and the normalization integral the mean energy can be simplified to:

$$\langle E_n \rangle = (n+\tfrac{1}{2}) + \frac{\tfrac{1}{2}\int_{-\infty}^{+\infty} \theta'(a,b)^2 \psi_n^2(x)dx}{\int_{-\infty}^{+\infty} \psi_n^2(x)\theta(a,b)dx} \qquad 30$$

The integral with $\theta'(a,b)^2$ must be simplified before equation 30 can be evaluated. First, $\theta'(a,b)^2$ can be replaced by $\theta'(a,b)$ as both series have the same limit. $\theta(a,b)$ is similar to the step function $S(x-a)$ (equal to zero for all x less than a and one for all x greater than or equal to a), that is it represents the two endpoints of the Heaviside function. The step function has a known derivative, the Dirac delta function defined by:

$$\int_{-\infty}^{+\infty} \delta(x-a)f(x) = f(a) \qquad 31$$

$f(x)$ has the same properties as in equation 27. Then, by analogy, $\theta'(a,b) = \delta(x-a) + \delta(x-b)$, and therefore:

$$\int_{-\infty}^{+\infty} \theta'(a,b)^2\psi_n^2(x)dx = \psi_n^2(a) + \psi_n^2(b) \qquad 32$$

If the harmonic oscillator is considered to be symmetrical, i.e. $-a \leq x \leq a$, then the mean energy becomes:

$$\langle E_n \rangle = (n+\tfrac{1}{2}) + \psi_n^2(a) / \int_{-a}^{+a} \psi_n^2(x)dx \qquad 33$$

The second term of the equation represents the contribution due to the endpoint of the wave function. For large a $\psi_n(a)$ approaches zero and the integral approaches unity, so that the correct asymptotic energy is produced. For a going to zero, the integral goes to zero and the term becomes indeterminate. However, such a system has no physical meaning and can be discarded.

The effect of localization on the mean energy can be seen in figure one. Particulars of the classical case are found in table one. The interesting feature of figure one is the energy spectrum given by $E_n - E_{n-1}$. As the domain for the various states is lessened this quantity becomes slightly less than unity. This slight crowding of states is also a feature present in the other methods of localization and appears to be a characteristic of the harmonic oscillator.

The kinetic energy has an interesting variation as the degree of localization is increased. The kinetic energy becomes negative just before the classical bound and remains thus until infinity. As the oscillator becomes localized, the negative part of the kintic energy is cut off. It then reaches a maximum at the zero point. After this the Heisenberg uncertainty principle fails to hold as both Δx and Δp go to zero.

The essential difficulty in this approach is the definition of the products of distributions. In considering the uncertainty in energy of these local states, products are created containing Heaviside functions to the third and fourth derivative. These can not be simplified by equation 27 and there is no intuitive meaning to the products so that the solutions can be evaluated. Numerical methods, using series, are usually divergent. An attempt was made to overcome this difficulty by using the closure relationship:

$$1 = \sum_{v} |\phi_v\rangle\langle\phi_v| \tag{34}$$

$$\langle E_n\rangle = \langle\Psi_n|H|\Psi_n\rangle \tag{35}$$

$$= \sum_{v} \langle\Psi_n|H|\phi_v\rangle\langle\phi_v|\Psi_n\rangle \tag{36}$$

ϕ_v is considered to represent the set of eigenfunctions of the harmonic oscillator for the infinite domain. The mean energy can be written as:

$$\langle E_n \rangle = E_n \, |\langle \Psi_n | \phi_n \rangle|^2 + \sum_{v \neq n} E_v \, |\langle \Psi_n | \phi_v \rangle|^2 \qquad 38$$

This method is not satisfactory as the summation term becomes divergent for fairly localized systems.

Another method of overcoming the problem of evaluating products of distributions is to transform the wave function into momentum space. Thus:

$$\Psi(p) = \frac{1}{\sqrt{2\pi}} N \int_{-\infty}^{+\infty} \psi(x)\theta(a,b)e^{ip.x}dx \qquad 39$$

The mean kinetic energy is then given by:

$$\langle p^2 \rangle = \int_{-\infty}^{+\infty} \Psi(p)p^2\Psi(p)dp \qquad 40$$

The integrals of 39 and 40 can not be solved analytically, and in using numerical techniques the wave function in momentum space is found to be weakly convergent. This is a basic property of the Fourier transform. As the wave packet becomes sharply defined in position space the momentum wave packet starts to spread and oscillate sinusoidally. This feature,noticeable in the kinetic energy starting about forty atomic units, causes it to be divergent for small values of a, the boundary value in position space. Consequently, calculations involving the uncertainty in energy can not be made.

The wave function used for these calculations is only an approximation to the solution of the Schrodinger equation on a bounded interval as the eigenfunctions for the infinite domain were used. The approximation then becomes more gross as the domain becomes small. This can be seen directly from the wave function, which looks cut up at the endpoint. A more rigorous approach in which the Schrodinger equation is solved for a bounded interval is developed in the next section. The problem of distributions does not occur.

FIGURE 1. Variation of the mean energy of the local harmonic oscillator with change in the radius of localization for the first four states. The mean energy is calculated using equation 33, with the classical limit given by $E = \frac{1}{2}x^2$ drawn in.

FIGURE 1

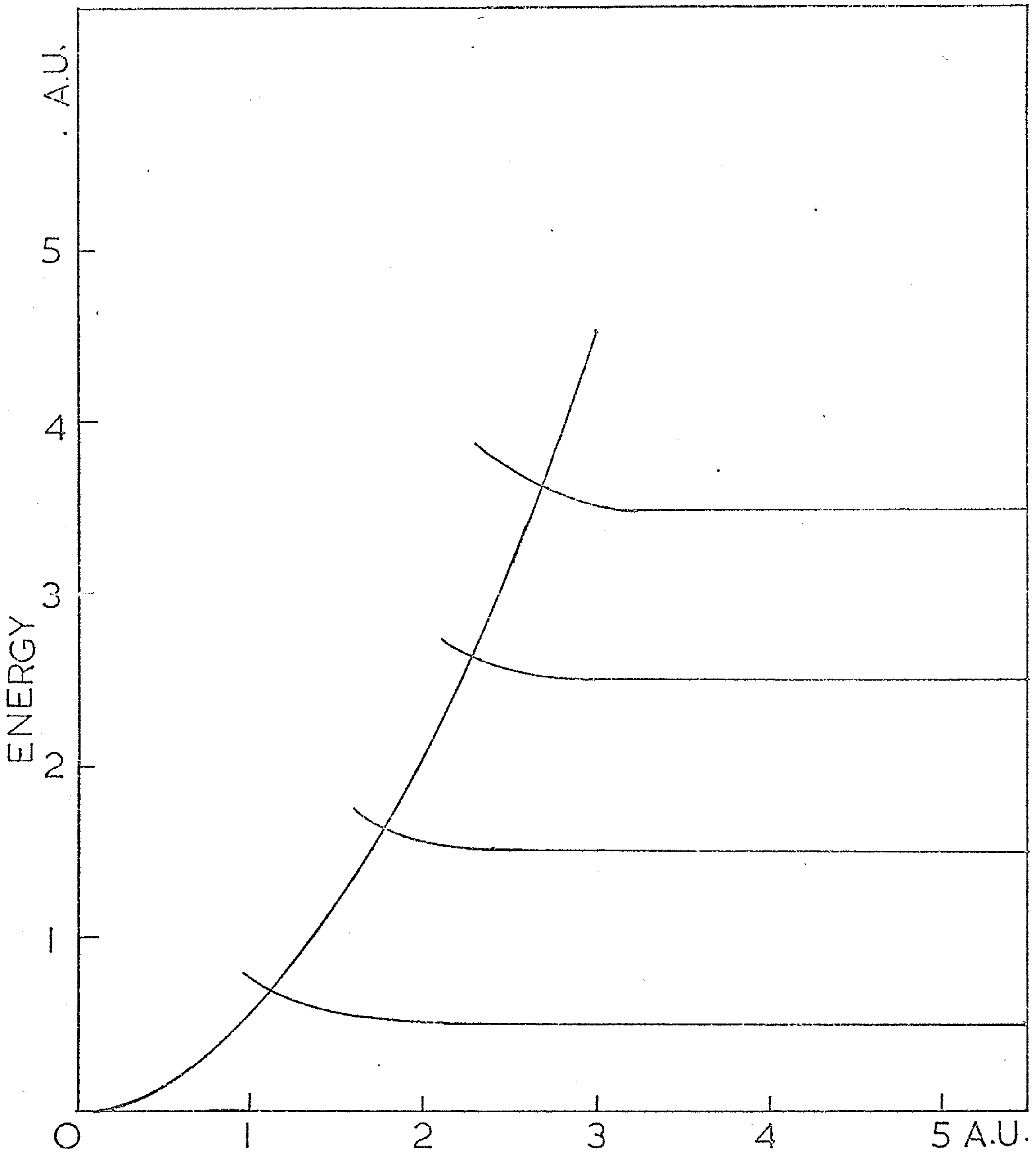


FIGURE 2. Plot of the ground state wave function localized on a domain between ±1.5 a.u. . Equation 5 is used. For a comparison to a non-localized wave function see figure 4, page 27.

FIGURE 2

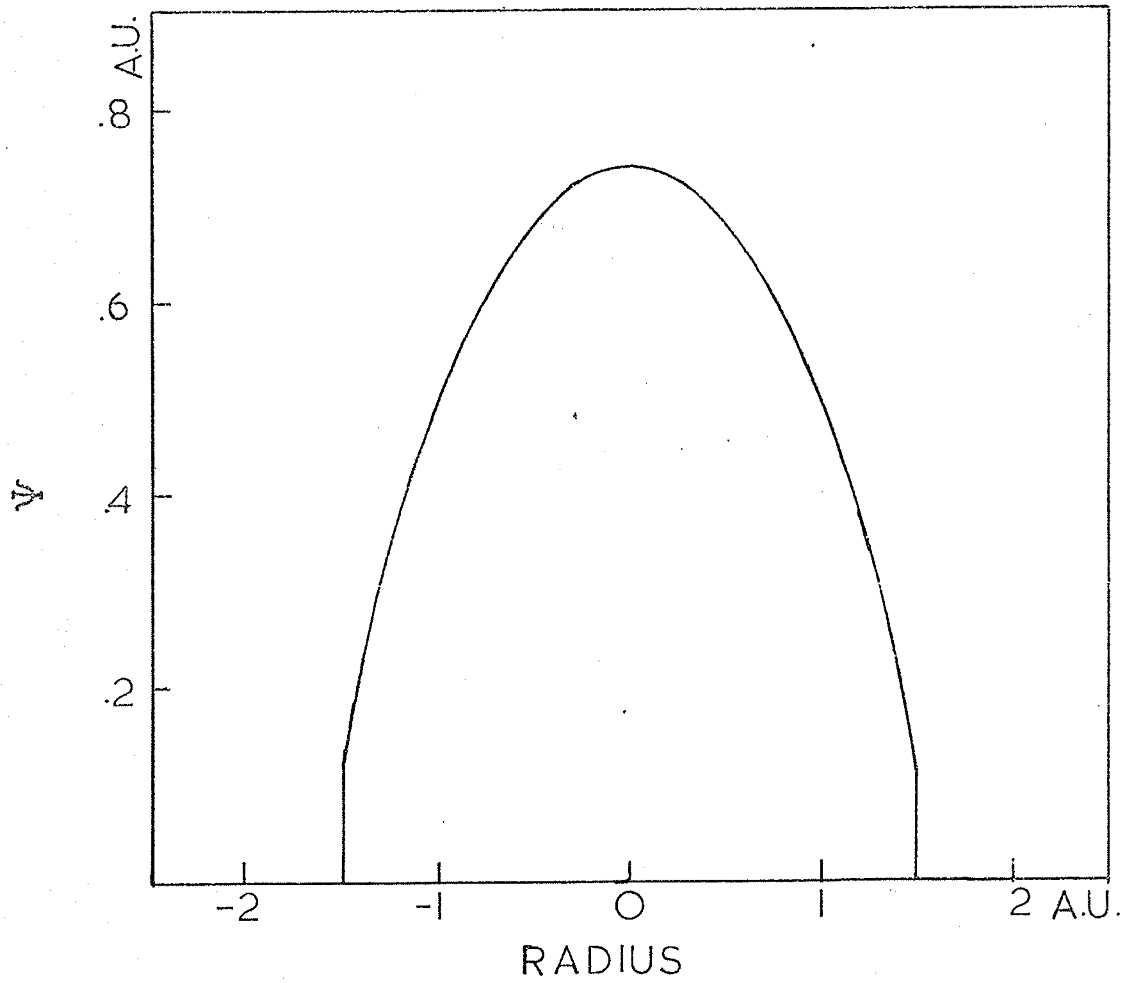


TABLE I

MEAN ENERGIES AND UNCERTAINTIES FOR THE FIRST SEVEN STATES LOCALIZED ON THE CLASSICAL DOMAIN (CALCULATED IN ATOMIC UNITS USING DISTRIBUTION THEORY)

STATE	CLASSICAL RADIUS		ENERGIES		$E_n - E_{n-1}$
		KINETIC	POTENTIAL	MEAN	
0	1.1541	1.0235	0.3085	0.6660	
1	1.8167	2.0235	1.2272	1.6502	0.9842
2	2.2987	3.1245	2.1594	2.6420	0.9917
3	2.6968	4.1734	3.0992	3.6363	0.9944
4	3.0437	5.2201	4.0441	4.6321	0.9957
5	3.3552	6.2647	4.9926	5.6286	0.9966
6	3.6403	7.3076	5.9439	6.6258	0.9971
7	3.9047	8.3490	6.8976	7.6233	0.9976

STATE	CLASSICAL RADIUS		UNCERTAINTIES	
		MOMENTUM	POSITION	PRODUCT
0	1.1541	1.0117	0.5554	0.5619
1	1.8167	1.4399	1.1078	1.5950
2	2.2987	1.7676	1.4695	2.5975
3	2.6968	2.0429	1.7605	3.5965
4	3.0437	2.2848	2.0110	4.5946
5	3.3552	2.5029	2.2344	5.5926
6	3.6403	2.7033	2.4380	6.5906
7	3.9047	2.8894	2.6263	7.5887

HARMONIC OSCILLATOR IN A POTENTIAL BOX

The Schrodinger equation (equation 20) can be solved for a bounded interval. However, as Schrodinger (28) noted, there are an infinite number of solutions to the equation since a new wave function and energy must be generated each time the domain is varied. Furthermore, the solution is not analytical, but must be solved by some series. In order to produce the correct asmyptotic energy it is necessary to stipulate a zero endpoint for the wave function. Otherwise a series can not be found to satisfy equation 20. The solutions may be written in terms of two Fourier series (36), one for the even states and one for the odd states.

$$\Psi_e(x) = \sum_n c_n \cos\ (n\pi x/2a) \qquad 41$$

$$\Psi_o(x) = \sum_n c_n \sin\ (n\pi x/a) \qquad 42$$

A symmetrical oscillator is required with the bound given by $\pm a$. n has to be an odd positive integer for the even states to have a zero endpoint. For the odd states, n is a positive integer. The Fourier coefficients 'c_n' have to be obtained before the wave function becomes known. This is accomplished by converting the function to a matrix, and evaluating the energy matrix. The eigenvectors obtained from the diagonalization are the Fourier coefficients desired. The detailed evaluation of the integrals appear in appendix B; only the final result will be stated in the thesis proper. Equation 22 is used to perform the calculations.

Even state calculations of normalization, kinetic and potential energy

$$\langle \Psi_e | \Psi_e \rangle = \sum_{n,m} c_n c_m \int_{-a}^{+a} \cos\ (n\pi x/2a)\ \cos\ (m\pi x/2a)\ dx \qquad 43$$

$$\langle \Psi_e | \Psi_e \rangle = a \sum_{m,n} c_n^2 \delta_{nm} \qquad 44$$

δ_{nm} is the kronecker-delta symbol ($\delta_{nm} = 1$ for $m = n$; zero for $m \neq n$).

$$\langle \Psi_e | p^2 | \Psi_e \rangle = \frac{\pi^2}{4a^2} \sum_{m,n} c_n c_m n^2 \int_{-a}^{+a} \cos(m\pi x/2a)\cos(n\pi x/2a)dx \qquad 45$$

$$= \frac{\pi^2}{4a} \sum_{m,n} n^2 c_n^2 \delta_{nm} \qquad 46$$

$$\langle \Psi_e | x^2 | \Psi_e \rangle = \sum_{m,n} c_n c_m \int_{-a}^{+a} x^2 \cos(n\pi x/2a)\cos(m\pi x/2a)dx \qquad 47$$

$$= a^3 \sum_{m,n} c_n \left[\frac{1}{3} + \frac{2\cos(n\pi)}{(n\pi)^2}\right] \delta_{nm} \; +$$

$$2a \sum_{m \neq n} c_n c_m \left[\frac{\cos\,(m+n)\pi/2}{\left((m+n)\pi/2\right)^2} + \frac{\cos\,(m-n)\pi/2}{\left((m-n)\pi/2\right)^2}\right] \qquad 48$$

The energy matrix $\langle \Psi_e | H | \Psi_e \rangle$ is given by:

$$\frac{\pi^2}{8a} \sum_{m=n} c_n^2 n^2 + \frac{a^3}{2} \sum_{m=n} c_n^2 \left[\frac{1}{3} + \frac{2\cos(n\pi)}{(n\pi)^2}\right] \; +$$

$$a \sum_{m \neq n} c_n c_m \left[\frac{\cos\,(m+n)\pi/2}{\left((m+n)\pi/2\right)^2} + \frac{\cos\,(m-n)\pi/2}{\left((m-n)\pi/2\right)^2}\right] \; =$$

$$Ea \sum_{m=n} c_n^2 \qquad 49$$

Differentiating with respect to c_k to minimize the energy, and sorting terms, a set of simultaneous linear equations is generated for each value of k. The energy matrix is:

$$\sum_n c_n \left\{ \frac{\pi^2 k^2}{8\,a^2} \delta_{kn} + \frac{a^2}{2}\left[\frac{1}{3} + \frac{2\cos(k\pi)}{(k\pi)^2}\right]\delta_{kn} - E\,\delta_{kn} \; + \right.$$

$$a^2\left[\frac{\cos[(k+n)\pi/2]}{[(k+n)\pi/2]^2}+\frac{\cos[(k-n)\pi/2]}{[(k-n)\pi/2]^2}\right](1-\delta_{kn})\Bigg\}=0 \qquad 50$$

Similarly, the energy matrix for the odd states is:

$$\sum_n c_n\left\{\frac{\pi^2k^2}{2a^2}\,\delta_{kn}+\frac{a^2}{4}\left[\frac{2}{3}-\frac{1}{(k\pi)^2}\right]\delta_{kn}-E\,\delta_{kn}+\right.$$

$$\left.a^2\left[\frac{\cos[(k-n)\pi]}{[(k-n)\pi]^2}-\frac{\cos[(k+n)\pi]}{[(k+n)\pi]^2}\right](1-\delta_{kn})\right\}=0 \qquad 51$$

To determine the classical bound, $\frac{1}{2}a^2$ is substituted for the energy in equations 50 and 51 and the resulting determinant is evaluated for all boundary values that cause it to vanish.

Table 2 indicates the characteristics of the classically bound system. The energy spectrum is similar to that of the distribution theory approach; only it is not as closely spaced for the lower states. It is extremely difficult to investigate this spacing with the previous approach. With the oscillator in a potential box, such spacing could depend upon the order of the matrix and the type of functions that were originally used. However, there is no variation of the energy when the matrix size is changed from fifty to ninety. The Fourier series used though could be considered incomplete. To test such a hypothesis the ground state wave function was written as:

$$\Psi_e(x)\sim\cos(n\pi x/2a)+\sin^2(n\pi x/a) \qquad 52$$

n is still a positive odd integer so that the boundary condition remains satisfied. With the wave function in this form, there are off-diagonal overlap terms. Special techniques (37) are required for diagonalizing a matrix with energy terms on the off-diagonals. The matrix for equation 52 can be subdivided into four smaller matrices representing the cosine, sine, and cosine-sine cross terms. As more terms are added to the sine matrix, the simultaneous equations become singular and the energy matrix can not be diagonalized. The only other set of functions that could adequately describe the wave function is a complex Fourier series. This is developed in the last part of the thesis and has to be given special attention to account for the alternating parity of the eigenfunctions. Thus the question of the spacings of the energy levels appears to be a property of the system.

As with the distribution theory approach, the oscillator in a box produces the expected results of localized systems. The energy variations are shown in figure three. The classically localized wave functions are plotted in figures four to six in comparison to the infinite domain case. All wave functions are normalized. The product of uncertainty tends to $(n+\frac{1}{2})\hbar$ for the upper classically localized functions as their domain becomes large and contains most of the wave function. The uncertainty in energy is zero for the spectrum as the matrix was transformed into the energy representation.

The transition spectrum can also be calculated by the usual methods (38). As the domain for the lower state is smaller than the upper state, the boundary of the lower one is used as the limits of the transition integral. For large values of the boundary, both qualitative and quantitative results are obtained. For the classically localized case, the integrals give only a qualitative answer as to the transitions allowed. To obtain a more quantitative answer perturbation theory was employed. In diagonalizing the energy matrix for the lower state, a set of upper levels were also obtained for this particular domain. This is true of the next classically localized state. When perturbation theory was used to consider the possibility of virtual transitions between these extra states, either an over or under complete set of states was used. Neither case yielded quantitative results similar to the transition spectrum of the infinite domain case.

Although this method is more rigorous than the previous approach it is awkward as large matrices of eigenvectors are required for each boundary value of a. Furthermore, there can be the problem of the set of functions not being complete, especially if the method is extended to a three dimensional model. The wave function, though, can be circumvented by considering a completely numeric approach, such as a finite difference one. This method will be developed in the next section.

TABLE II

MEAN ENERGIES AND UNCERTAINTIES FOR THE FIRST SEVEN STATES LOCALIZED ON THE CLASSICAL DOMAIN (CALCULATED IN ATOMIC UNITS BY SOLVING THE SCHRODINGER EQUATION)

STATE	CLASSICAL RADIUS	KINETIC	ENERGIES POTENTIAL	MEAN	E_n-E_{n-1}
0	1.2968	0.7363	0.1045	0.8408	
1	1.9163	1.3695	0.4667	1.8361	0.9954
2	2.3811	1.9817	0.8532	2.8349	0.9980
3	2.7693	2.5813	1.2531	3.8344	0.9994
4	3.1094	3.1721	1.6620	4.8341	0.9997
5	3.4158	3.7566	2.0773	5.8339	0.9998
6	3.6970	4.3361	2.4977	6.8338	0.9999
7	3.9582	4.9116	2.9222	7.8337	0.9999

STATE	CLASSICAL RADIUS	UNCERTAINTIES MOMENTUM	POSITION	PRODUCT
0	1.2968	1.2135	0.4571	0.5546
1	1.9163	1.6549	0.9661	1.5989
2	2.3811	1.9908	1.3063	2.6006
3	2.7693	2.2721	1.5831	3.5970
4	3.1094	2.5188	1.8232	4.5922
5	3.4158	2.7410	1.2038	5.5870
6	3.6970	2.9449	2.2350	6.5819
7	3.9582	3.1342	2.4175	7.5769

FIGURE 3. Variation of the mean energy of the local harmonic oscillator with change in the radius of localization for the first six states. The mean energy is calculated using equations 50 and 51, with the classical limit given by $E = \frac{1}{2}x^2$ drawn in. Within the classical bound the energy of the various states rises asymptotically as the domain is localized. This is not shown as it is not physically meaningful to consider a state so localized. This energy trend is present, but not shown, in the other energy spectrum figures.

FIGURE 3

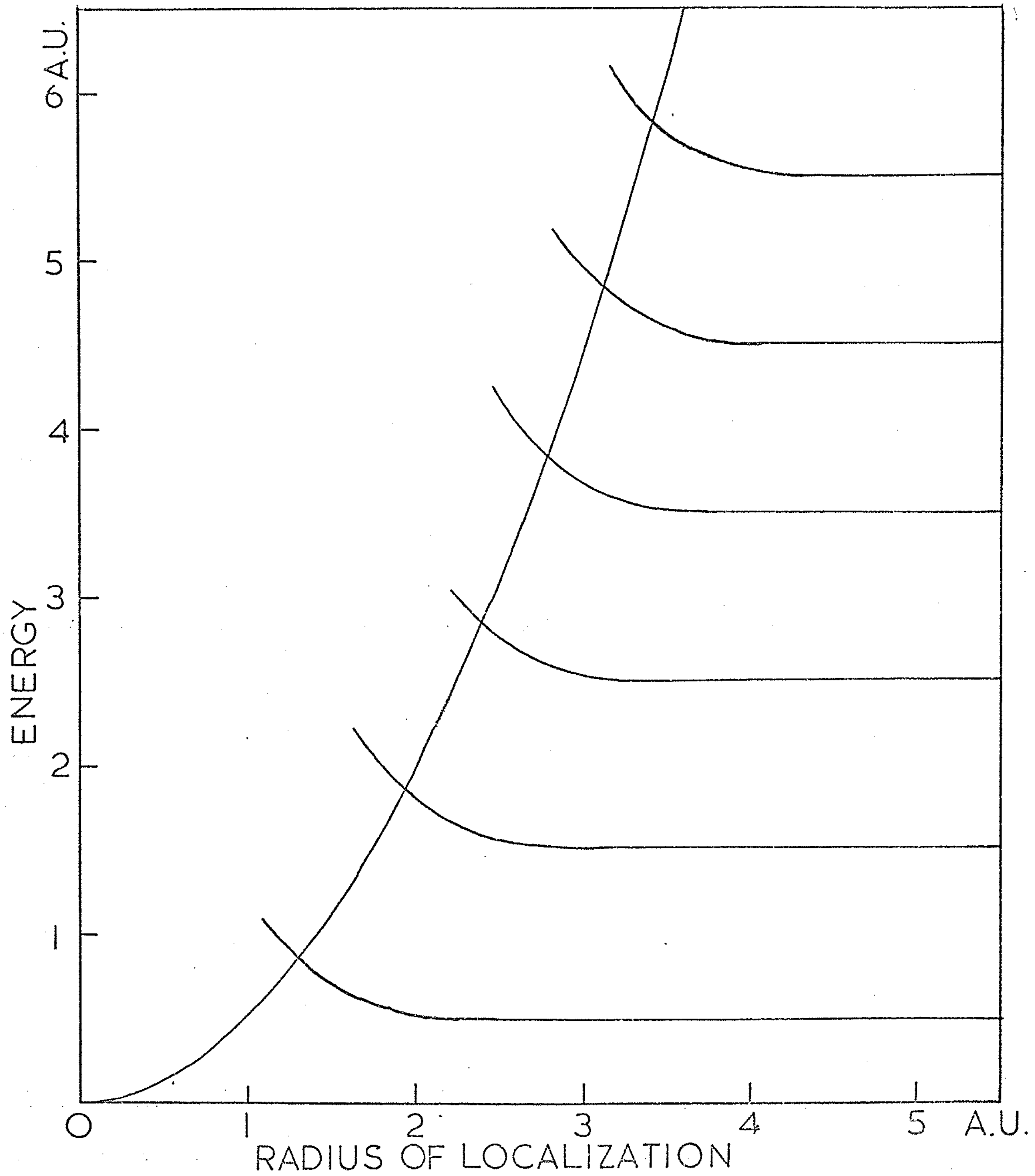


FIGURE 4. Plot of the ground state wave function. The upper graph represents the wave function of the infinite domain while the lower graph represents the wave function of the classical domain case. Equation 41 was used. The classical domain is given by the value of a, the boundary value, where the energy of the state is intersected by the energy given by $\frac{1}{2}x^2$.

FIGURE 4

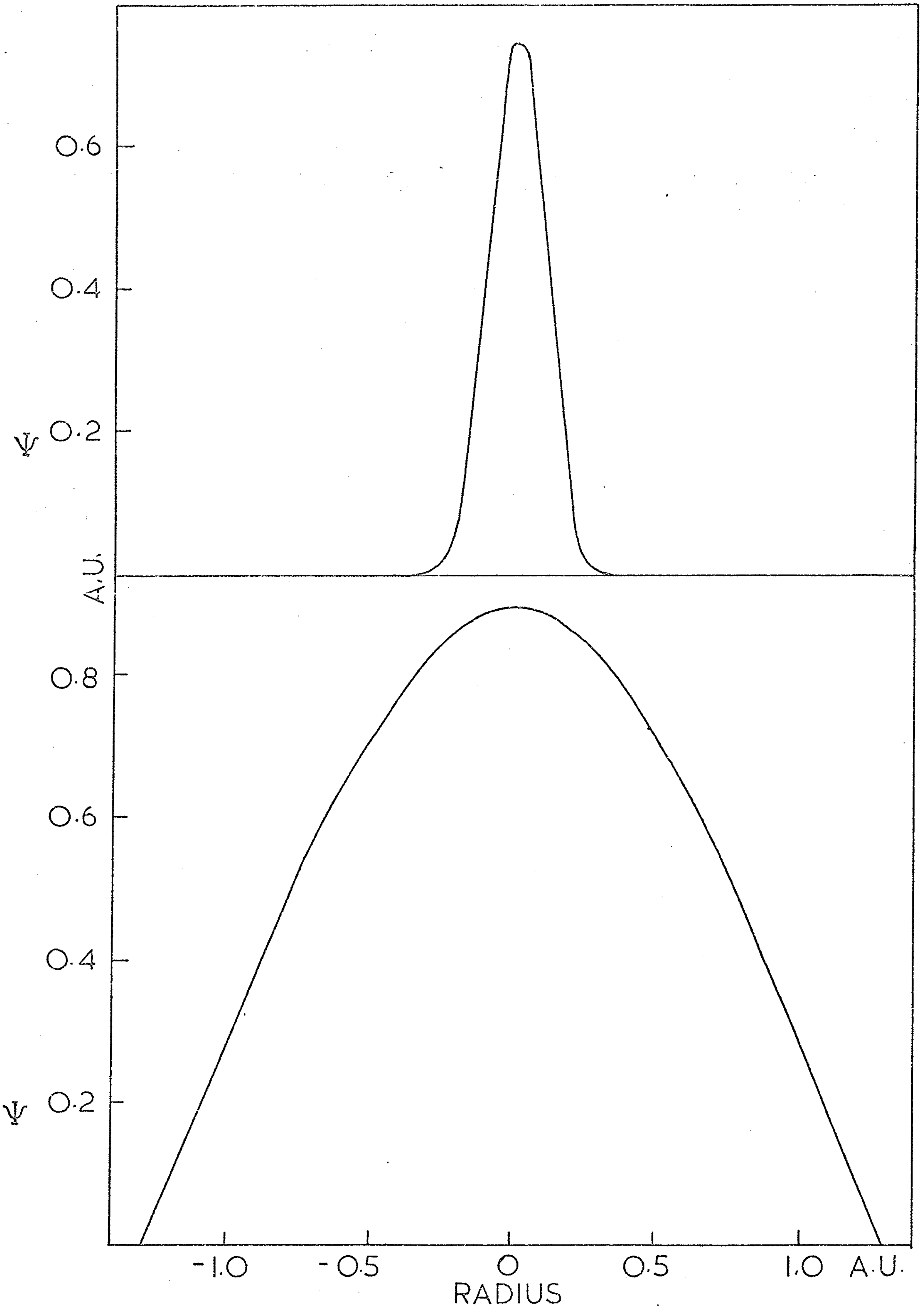


FIGURE 5. Plot of the wave function for the first excited state. The upper graph represents the wave function of the infinite domain while the lower graph represents the wave function of the classical domain case. Equation 42 was used.

FIGURE 5

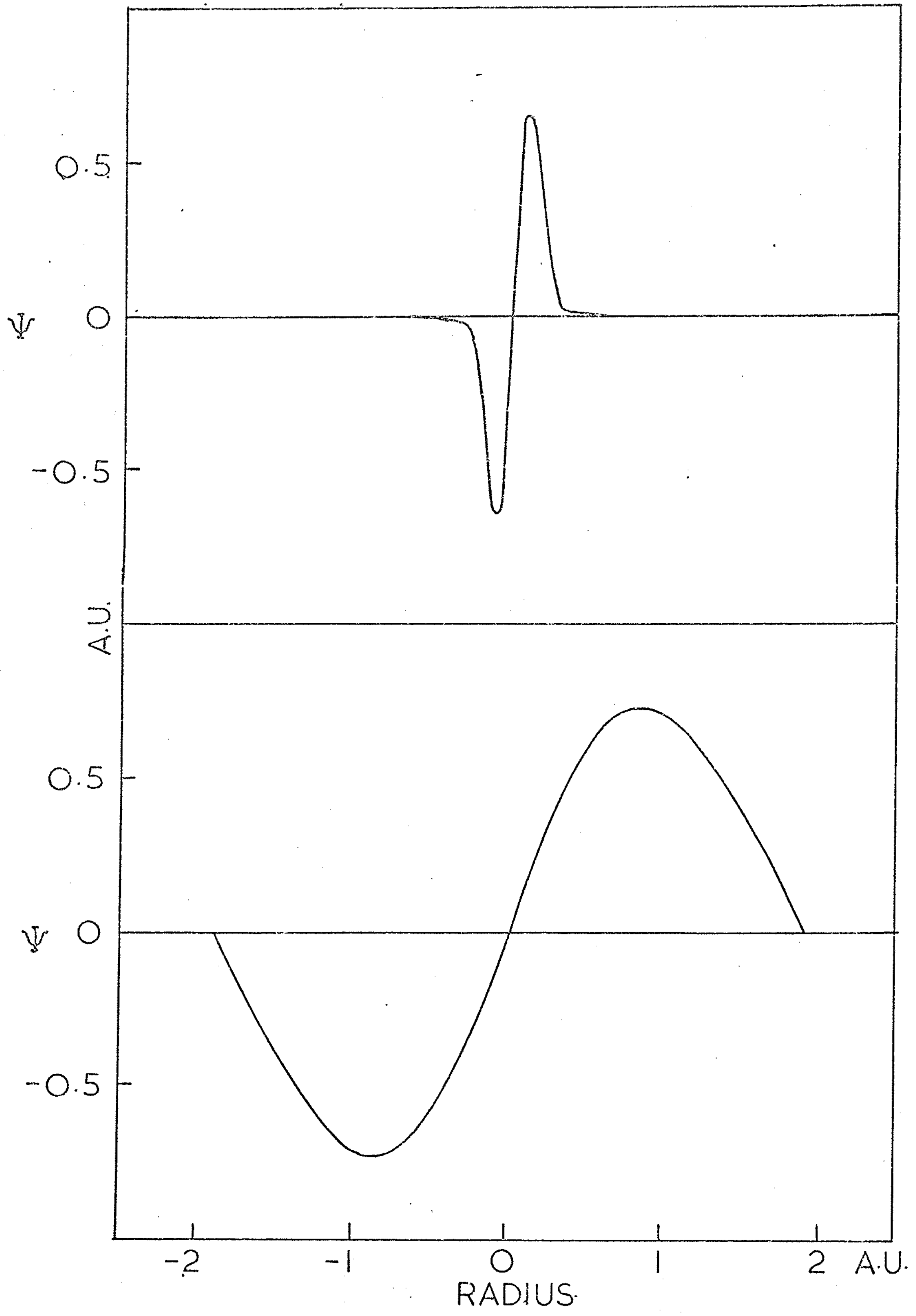
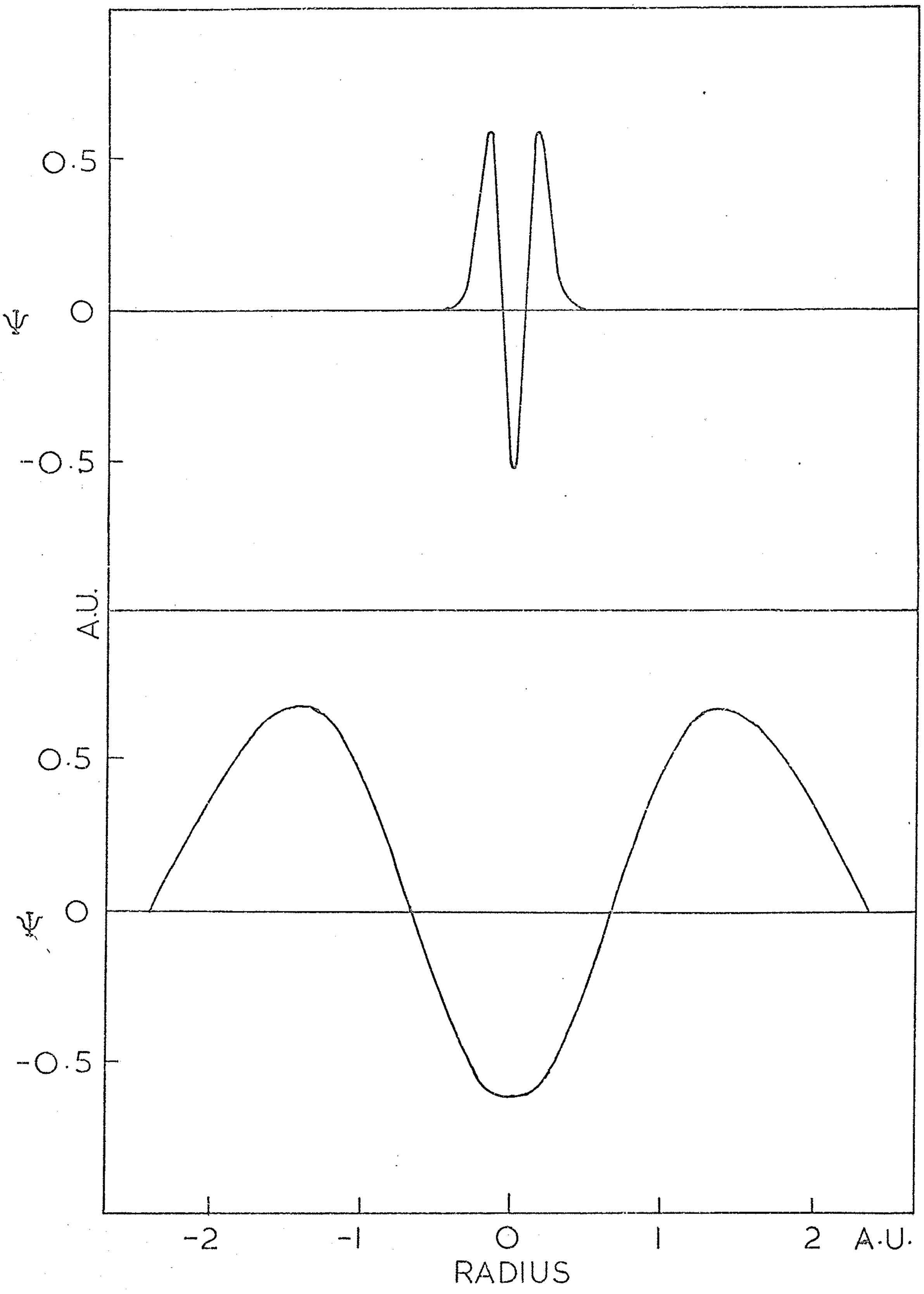


FIGURE 6. Plot of the wave function for the second excited state. The upper graph represents the wave function of the infinite domain while the lower graph represents the wave function of the classical domain case. Equation 41 was used

FIGURE 6



FINITE DIFFERENCE METHOD

The localized harmonic oscillator can be solved without recourse to any analytical function or series. This method, completely numeric, makes no assumption of the form of the eigenfunction except that it have a zero endpoint. The method generates a set of points that approximates the wave function. As more points are generated, the net of points better approximates the function. This method is called the finite difference method (39). The basic form of the equation used is:

$$L\Psi_j + E\Psi_j = 0 \qquad 53$$

L is an approximation to the Hamiltonian; E is the energy of the system; and Ψ_j represents the value of the wave function corresponding to some x_j point. Equation 53 is a matrix equation and if some value for the operator L is found it can be diagonalized to give the energy levels for the harmonic oscillator. To make the calculations easier, it is made symmetrical. L has the form:

$$L = -\tfrac{1}{2}\,\frac{1}{h}\left[\frac{\Psi_{j+1} - \Psi_j}{h} - \frac{\Psi_j - \Psi_{j-1}}{h}\right] + \tfrac{1}{2}x_j^2\Psi_j \qquad 54$$

The basic definition of a derivative is used. As h goes to zero, the true derivative will be achieved. This requires that the j^{th} index number become large. The axis points are given by:

$$x_j = -a + jh \qquad 55$$

h is the interval by which each point is augmented. The index factor j ranges from 0, to J + 1. This gives h a value of:

$$h = 2a/(J + 1) \qquad 56$$

Simplifying equation 54:

$$L = -\frac{1}{2h^2}\left[\Psi_{j+1} + \Psi_{j-1} - 2\Psi_j\right] + \frac{1}{2}x_j^2\Psi_j \tag{57}$$

$$= -\frac{1}{2h^2}\Psi_{j+1} - \frac{1}{2h^2}\Psi_{j-1} + \frac{1}{2}(x_j^2 + \frac{2}{h^2})\Psi_j \tag{58}$$

The wave function is now defined by:

$$\Psi = \begin{bmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_J \end{bmatrix} \tag{59}$$

Ψ_0 and Ψ_{J+1} have been defined as zero. The index factor now goes only between 0 and J. A matrix equation has now been formed defined in the following manner:

$$L_{j,j-1} = -\tfrac{1}{2} \tag{60a}$$

$$L_{j,j+1} = -\tfrac{1}{2} \tag{60b}$$

$$L_{j,j} = \tfrac{1}{2}(x_j^2 + 2/(h^2) \tag{60c}$$

The matrix equation 53 is now written as:

$$(L_{j,j-1}, L_{j,j}, L_{j,j+1}) \begin{bmatrix} \Psi_{j-1} \\ \Psi_j \\ \Psi_{j+1} \end{bmatrix} = Eh^2 \begin{bmatrix} \Psi_{j-1} \\ \Psi_j \\ \Psi_{j+1} \end{bmatrix} \tag{61}$$

The problem of finding the energy levels only consists in diagonalizing matrix L. This is a symmetric tridiagonal matrix with all other values put to zero. To acheive a high degree of accuracy the order of the matrix must become very large. Table three indicates the change in energy as the order is increased.

These numbers are for the classically localized particle. It is not possible to evaluate the upper states accurately as the order of the matrix becomes too large for the computer to handle. The variation of the energy with the boundary of the domain is shown in figure seven. As the matrix size becomes large, this method coincides with the oscillator in a box approach. The method can be improved by taking the approximations to a higher order. This has the effect of increasing the effective matrix size. In using this method without higher order terms in the matrix, the energy has an upper bound, while with them the energy approaches a lower bound. The true energy occurs when these two bounds meet.

This procedure is a powerful technique if a suitable wave function can not be readily found to describe the state, that is, molecules and many electron atoms whose wave functions are obtained in a self-consistent manner. However, there are basic difficulties with this method that are not present in the harmonic oscillator. There are no singularities in the differential equation as there are in the hydrogen atom or helium atom. These points require special computer techniques as the concepts of infinity and division by zero are not easily programmed.

Furthermore, the wave function is sacrificed for a set of points approximating it. These are the eigenvectors that come from diagonalizing the energy matrix. To obtain a normalized wave function requires that the points be plotted against the corresponding x_j points. The area under the curve is then found and this number divides the eigenvector to normalize it. The mean parameters require a similar amount of manipulation. To evaluate the mean potential energy, the eigenvector is multiplied by the corresponding x_j^2 and the points are numerically integrated. The mean kinetic is found by subtracting the mean potential energy from the mean energy. Otherwise, a numeric method for differentiating each point must be used. The eigenvectors were found to be identical to the corresponding wave functions of the oscillator in a box method and are not shown. The other mean parameters for the finite difference method were also found to correspond to the previous approach.

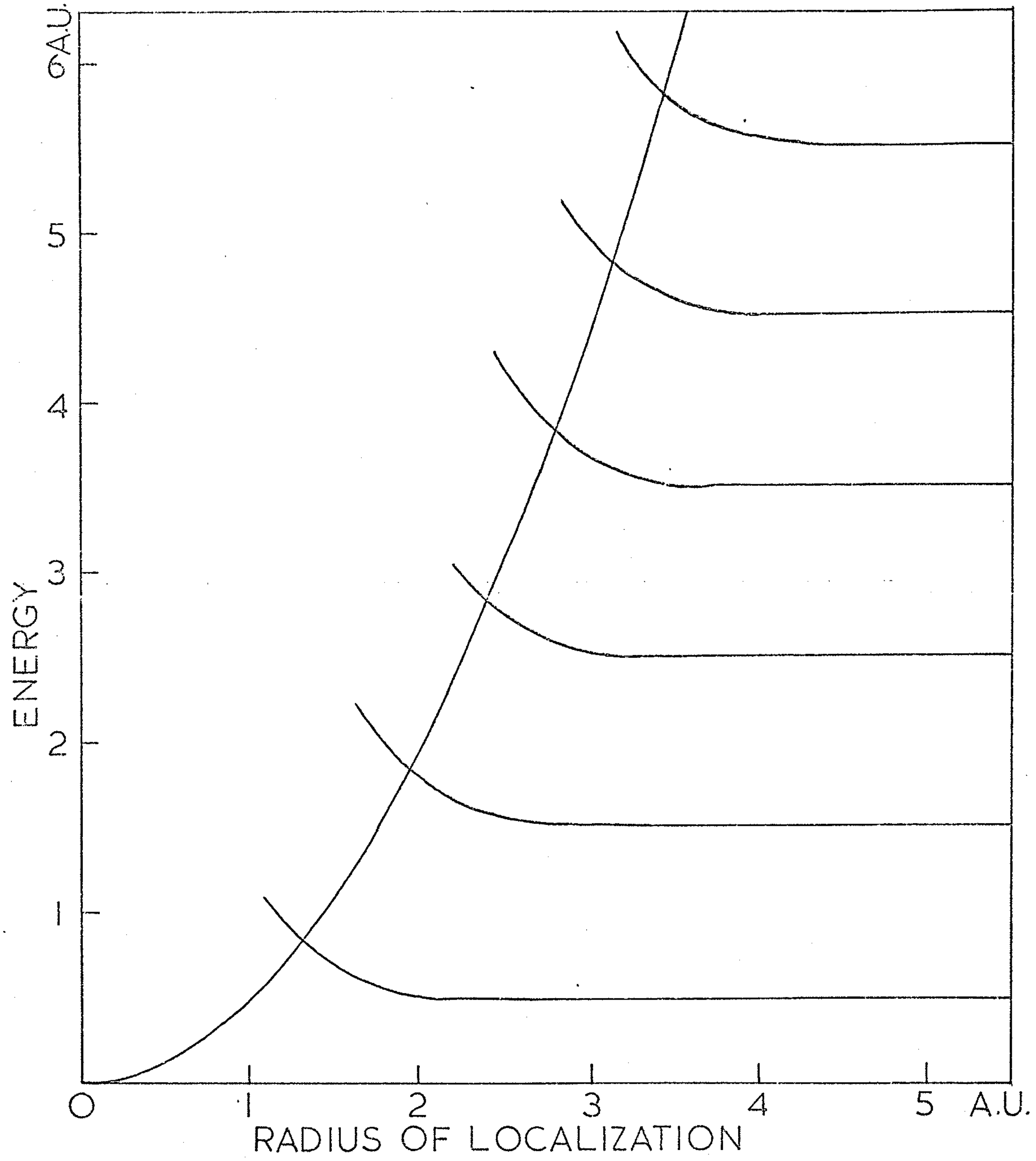
TABLE III

MEAN ENERGIES OF THE FIRST FOUR STATES LOCALIZED ON THE CLASSICAL DOMAIN AS A FUNCTION OF MATRIX SIZE (CALCULATED IN ATOMIC UNITS USING A FINITE DIFFERENCE METHOD)

MATRIX ORDER	STATE	CLASSICAL RADIUS	ENERGY	$E_j - E_{j-1}$
100	0	1.2967	0.8406	
200	0	1.2967	0.8407	
	1	1.9162	1.8360	0.9953
	2	2.3810	2.8346	0.9988
	3	2.7690	3.8337	0.9991
600	0	1.2968	0.8408	
	1	1.9163	1.8361	0.9953
	2	2.3811	2.8349	0.9987
	3	2.7692	3.8341	0.9992

FIGURE 7. Variation of the mean energy of the local harmonic oscillator with the radius of localization for the first four states. The mean energy is calculated using equation 61 with the classical limit given by $E = \frac{1}{2}x^2$ drawn in.

FIGURE 7



VON NEUMANN OR BOUNDED OPERATOR APPROACH

In the previous sections more emphasis was placed upon a localized wave packet. This section evaluates the eigenfunction derived from a bounded operator with no restrictions placed upon it. In considering a symmetric oscillator, von Neumann's wave function becomes:

$$\Psi(x) = \frac{1}{\sqrt{2a}} e^{-i\pi(\alpha/2\pi + k)x/a} \qquad k = 0 \pm 1 \pm 2 \ldots \qquad 62$$

Alpha, which governs the hermitian nature of the operator also controls the parity of the various states. Equation 62 can have two extreme cases: with alpha equal to zero, odd states are generated; with alpha equal to pi, even states. These states will be shown to be identical to wave functions of the oscillator in a potential box. As alpha ranges between its two values a large number of functions are generated for each boundary value. There is no stipulation that the endpoints be zero or finite as the various alpha values will automatically determine this condition. However, as the boundary value a goes to infinity the endpoint goes to zero regardless of the value of alpha to give the correct asymptotic energy.

A different type of stipulation for accepting wave functions must be formulated as not all wave functions will be well behaved quantum mechanically. This stipulation is the Heisenberg uncertainty principle, that is the wave function must generate the correct mean energies so that the product of the uncertainties in position and momentun must be greater than or equal to $\frac{1}{2}\hbar$.

The eigenvalues and eigenvectors for equation 62 are generated in an analogous manner to the oscillator in a box. All the integrals will be evaluated in appendix c. The wave function is normalized as it stands and its complex conjugate is given by:

$$\Psi^*(x) = \frac{1}{\sqrt{2a}}\, e^{i\pi(\alpha/2\pi + k)x/a} \qquad 63$$

The kinetic energy is given by $\langle\Psi|p^2|\Psi\rangle$

$$\langle p^2\rangle = \frac{1}{2a}\left[\frac{\pi}{a}\left(\frac{\alpha}{2\pi}+k\right)\right]^2 \int_{-a}^{a} e^{i\pi(\alpha/2\pi+k)x/a}\, e^{-i\pi(\alpha/2\pi+l)x/a}\, dx \qquad 64$$

$$= \left[\frac{\pi}{a}\left(\frac{\alpha}{2\pi}+k\right)\right]^2 \delta_{kl} \qquad 65$$

The potential energy is given by $\langle\Psi|x^2|\Psi\rangle$

$$\langle x^2\rangle = \frac{1}{2a}\int_{-a}^{a} x^2\, e^{i\pi(\alpha/2\pi+k)x/a}\, e^{-i\pi(\alpha/2\pi+l)x/a}\, dx \qquad 66$$

$$= \frac{a^2}{3}\,\delta_{kl} + \frac{2a^2}{\pi^2}\frac{\cos[(k-l)\pi]}{(k-l)^2}(1-\delta_{kl}) \qquad 67$$

The energy matrix to be diagonalized is:

$$\frac{1}{2}\left[\frac{\pi}{a}\left(\frac{\alpha}{2\pi}+k\right)\right]^2 \delta_{kl} + \frac{a^2}{6}\,\delta_{kl} + \frac{a^2}{\pi^2}\frac{\cos[(k-l)\pi]}{(k-l)^2}(1-\delta_{kl}) - E\,\delta_{kl} = 0 \qquad 68$$

To plot the wave function and evaluate the mean parameters the wave function is written in the form:

$$\Psi(x) = \frac{1}{\sqrt{2a}}\sum_{-k}^{+k} c_k\, e^{i\pi(\alpha/2\pi+k)x/a} \qquad 69$$

c_k represents the eigenvectors obtained in diagonalizing the energy matrix.

Figures eight to ten show the varation of the energy with the boundary for three different values of alpha. These correspond to the two possible extreme values and an intermediate one. For alpha equal to zero and pi for the even and odd states respectively, there are minima that occur at the classical limit for all states except the lowest one. This state will be analyzed later. The other extreme case, alpha equal to zero and pi for the odd and even states respectively yield the same curves that were obtained in the oscillator in a box approach. These will be shown to be mathematically equivalent. The in between value is $\pi/2$. Alpha only affects the states near the classical bound where the curves take a slight dip. Data for the classical case are shown in table four for these values.

Particularly interesting is the lowest state with alpha equal to zero. Its energy goes to zero as it is localized. The explanation is found in the eigenvector. The coefficients are real and as a goes to zero, the ground state coefficient c_0, goes to one. For the vector to remain normalized, the remaining terms must vanish. Inspection of equation 65 shows that this part of the wave function is zero. Consequently the kinetic energy must vanish along with the potential energy so that $\Delta p \Delta x \rightarrow 0$ as $a \rightarrow 0$. An attempt was made to renormalize this vector by diminishing c_0 by a number less than unity and the remaining coefficients by a number greater than one. Numerically, this was equivalent to changing the value of alpha to be greater than zero. A similar attempt was made to remove this state by eliminating all $k = 0$ terms in the matrix to be diagonalized.

Although this removes the ground state vector, it also completely removes the ground state energy so that the lowest level is the first excited one. This particular wave function had to be discarded as it did not satisfy the Heisenberg uncertainty principle.

The wave function with $a = \pi/2$ possesses midway properties of the two extremes. This is reflected in the wave functions by their endpoints that vary between zero and some maximum. The states still retain their even/odd parity depending upon the state. As an example, for alpha going to pi for the first even state, the endpoints of the wave function slowly go to zero retaining its even parity. As this happens,the product of uncertainties becomes greater. By choosing the appropriate alphas, one can still generate an energy spectrum with spacings of unity, but the endpoints of the wave function will not be zero. These functions, however, are still quantum mechanical as they are square integrable,normalizable, and satisfy the eigenvalue equation.

The effect of alpha can be seen in figures eleven to thirteen for a classical radius of localization. For the wave function with the maximum at the endpoint, the kinetic energy is at a minimum and the potential energy is at a maximum. As alpha changes the uncertainty in position becomes less until it reaches its least value when the endpoints of the wave function are zero. Variations in the mean energies are graphed in figures fourteen to nineteen with their related uncertainties as a function of the radius of localization. Alpha directly affects the kinetic energy and causes it to be lowered for all alpha less than about 2/3 pi. This makes the product of the uncertainties of position and momentum become less than $\frac{1}{2}\hbar$ for many of the wave functions. Consequently, these can not be used as localized wave functions. Furthermore, the states are not desirable as the uncertainty in position becomes greater than that of the infinite domain case, and even though the particle is localized, one becomes too uncertain of where it is. However, although the kinetic energy becomes small, it does increase for very localized states to insure that the energy does not go to zero. These states are still not acceptable as the particle would be localized in a domain less than the classical one. Another conceptual point against these states is that there is no physical significance for eigenfunctions with the maxima at the endpoints. The more acceptable functions then appear to be those with the zero or near zero endpoint for their wave functions, that is they are derived by considering a bounded operator which has localized states and there is a corresponding small uncertainty in position associated with the particle. This uncertainty becomes less than that of the infinite domain state.

The wave function with the zero endpoints can be shown to correspond to the solutions of the oscillator in a box approach. The lowest even state will be used in the derivation, that is an alpha equal to pi. The odd states are proven to be identical in an analogous fashion. The function for the even states is:

$$\Psi(x) = \sum_{-k}^{+k} c_k \, e^{-i\pi(\frac{1}{2}+k)x/a} \qquad 70$$

$\Psi(x)$ is of even parity. Considering the oscillator to be symmetrical, multiplying by $e^{i\pi(\frac{1}{2}+k)x/a}$ and integrating, the coefficients have the value:

$$c_k = \int_{-a}^{+a} \Psi(x) \cos[(k-\tfrac{1}{2})\pi x/a]\,dx \qquad 71$$

The exponential term was split into sine and cosine terms and as the wave function is even the sine integral has zero area. Equation 71 indicates that the coefficients are real and that $c_k = c_{-(k+1)}$. $\Psi(x)$ can now be broken into two summations with the function expressed in terms of sines and cosines.

$$\Psi(x) = \sum_{k=-K}^{-1} c_k \Big[\cos[(k+\tfrac{1}{2})\pi x/a] - i \sin[(k+\tfrac{1}{2})\pi x/a]\Big] + \sum_{k=0}^{K} c_k \Big[\cos[(k+\tfrac{1}{2})\pi x/a] - i \sin[(k+\tfrac{1}{2})\pi x/a]\Big] \qquad 72$$

As the sine is an odd function, all but the K^{th} end sine term can be cancelled from equation 72. The wave function becomes:

$$\Psi(x) = 2\sum_{k=0}^{K}\Big[c_k \cos[(k+\tfrac{1}{2})\pi x/a]\Big] - i\, c_K \sin[(K+\tfrac{1}{2})\pi x/a] \qquad 73$$

As the matrix size is expanded to obtain a constant ground state energy the c_K coefficient tends to a small number and the imaginary part of equation 73 can be neglected. Consequently:

$$\Psi(x) = \sum_k c_k \cos(\pi kx/2a) \qquad 74$$

k is now an odd positive integer. The odd states for alpha zero can also be simplified to equation 42.

The odd wave function for a non-zero endpoint, that is an alpha of pi can be simplified to a real series of the form:

$$\Psi(x) = \sum_k c_k \sin(k\pi x/2a) \qquad 75$$

k is an odd positive integer. This simplification is not possible for the even state equivalent because the ground state does not cancel. The distribution for these states can be evaluated instead of the wave function. The odd state coefficients can be shown to be completely imaginary by a method analogous to that in deriving equation 71. Consequently, the product of the coefficients will always be real. The distribution is given by:

$$\Psi^*(x)\,\Psi(x) = \sum_{k,l} c_k c_l\, e^{-i\pi(\alpha/2\pi + k)x/a}\, e^{i\pi(\alpha/2\pi + l)x/a} \tag{76}$$

$$= \sum_{k,l} c_k c_l\, e^{-i\pi(k-l)x/a} \tag{77}$$

$$= \sum_{k,l} c_k c_l \Big[\cos[(k-l)\pi x/a] - i\,\sin[(k-l)\pi x/a]\Big] \tag{78}$$

For all $k = l$ terms the sine function is zero. Then the summation involving the sine can be written as:

$$\sum_{k \neq l} c_k c_l \sin[(k-l)\pi x/a] = \sum_{k>l} c_k c_l \sin[(k-l)\pi x/a] + \sum_{k<l} c_k c_l \sin[(k-l)\pi x/a] \tag{79}$$

For every off diagonal where there is a k greater than an l there is an off diagonal with the same coefficients but with l greater than k such that in one case (k-l) is a positive number and in the other (k-l) is the negative of the number. Consequently all the sine terms cancel. This is expected as all quantum mechanical distributions are real. The distribution then becomes:

$$\Psi^*(x)\,\Psi(x) = \sum_{k,l} c_k c_l \cos[(k-l)\pi x/a] \tag{80}$$

The distribution for the second state is shown in figure twenty for alpha equal to pi and one-half pi. The real function for alpha pi is shown in figure twenty-one, showing the non-zero endpoint.

The infinite domain and the classical domain wave functions were shown in the section on the oscillator in a potential box. The energy considerations are graphed here to show the trend of alpha on the mean parameters. This method basically represents the complex Fourier series solution for the oscillator in a box, that is, the even and odd state solutions were combined into a single function with a parameter to take into account the parity of the various states. The limitations of the previous approach are also present in this method. The derivation used by Von Neumann is a relatively simple one compared to that which has to be employed for the hydrogen atom. The hydrogen atom differential equation has to be solved using a different type of functions which take into account the natural singularities that occur in it. This is not completely without problems, as there are a large number of such functions.

TABLE IV

MEAN ENERGIES AND UNCERTAINTIES FOR THE FIRST FIVE STATES LOCALIZED ON THE CLASSICAL DOMAIN (CALCULATED IN ATOMIC UNITS BY THE VON NEUMANN APPROACH)

STATE	ALPHA	CLASSICAL RADIUS	ENERGIES			E_n-E_{n-1}
			KINETIC	POTENTIAL	MEAN	
0	π	1.2968	0.7363	0.1045	0.8408	
1	0	1.9163	1.3695	0.4667	1.8361	0.9954
2	π	2.3811	1.9817	0.8532	2.8349	0.9980
3	0	2.7693	2.5813	1.2631	3.8344	0.9994
4	π	3.1094	3.1721	1.6620	4.8341	0.9997

STATE	ALPHA	CLASSICAL RADIUS	UNCERTAINTIES		
			MOMENTUM	POSITION	PRODUCT
0	π	1.2968	1.2135	0.4571	0.5546
1	0	1.9163	1.6549	0.9661	1.5989
2	π	2.3811	1.9908	1.3063	2.6006
3	0	2.7693	2.2721	1.5831	3.5970
4	π	3.1094	2.5188	1.8232	4.5922

STATE	ALPHA	CLASSICAL RADIUS	ENERGIES			E_n-E_{n-1}
			KINETIC	POTENTIAL	MEAN	
0		not calculable for ground state				
1	π	1.5042	1.0879	1.1773	1.1261	
2	0	2.0703	2.1428	2.1443	2.1435	1.0173
3	π	2.5097	3.1485	3.1491	3.1488	1.0052
4	0	2.8816	4.1504	4.1504	4.1532	1.0097

TABLE IV CON'T

STATE	ALPHA	CLASSICAL RADIUS	UNCERTAINTIES		
			MOMENTUM	POSITION	PRODUCT
0		not calculable for ground state			
1	π	1.5042	1.0640	1.0634	1.1315
2	0	2.0703	1.4638	1.4643	2.1436
3	π	2.5097	1.7744	1.7747	3.1488
4	0	2.8816	2.0379	2.0372	4.1518

STATE	ALPHA	CLASSICAL RADIUS	KINETIC	POTENTIAL	MEAN	$E_n - E_{n-1}$
0	$\pi/2$	0.9764	0.6565	0.2985	0.4427	
1	$\pi/2$	1.7249	1.8094	1.1646	1.4870	1.0094
2	$\pi/2$	2.2320	2.9267	2.0541	2.4904	1.0034
3	$\pi/2$	2.6428	4.0280	2.9565	3.4923	1.0018
4	$\pi/2$	2.9978	5.1184	3.8683	4.4934	1.0011

STATE	ALPHA	CLASSICAL RADIUS	UNCERTAINTIES		
			MOMENTUM	POSITION	PRODUCT
0	$\pi/2$	0.9764	0.8103	0.5464	0.5547
1	$\pi/2$	1.7249	1.3451	1.0792	1.5988
2	$\pi/2$	2.2320	1.7108	1.4332	2.6005
3	$\pi/2$	2.6428	2.0070	1.7195	3.5970
4	$\pi/2$	2.9978	2.2624	1.9668	4.5922

FIGURE 8. Variation of the mean energy of the harmonic oscillator with the radius of localization for the first six states. The mean energy is calculated by using equation 68 with alpha zero for the even states and pi for the odd states. The classical limit is drawn in and all parameters are expressed in atomic units.

FIGURE 8

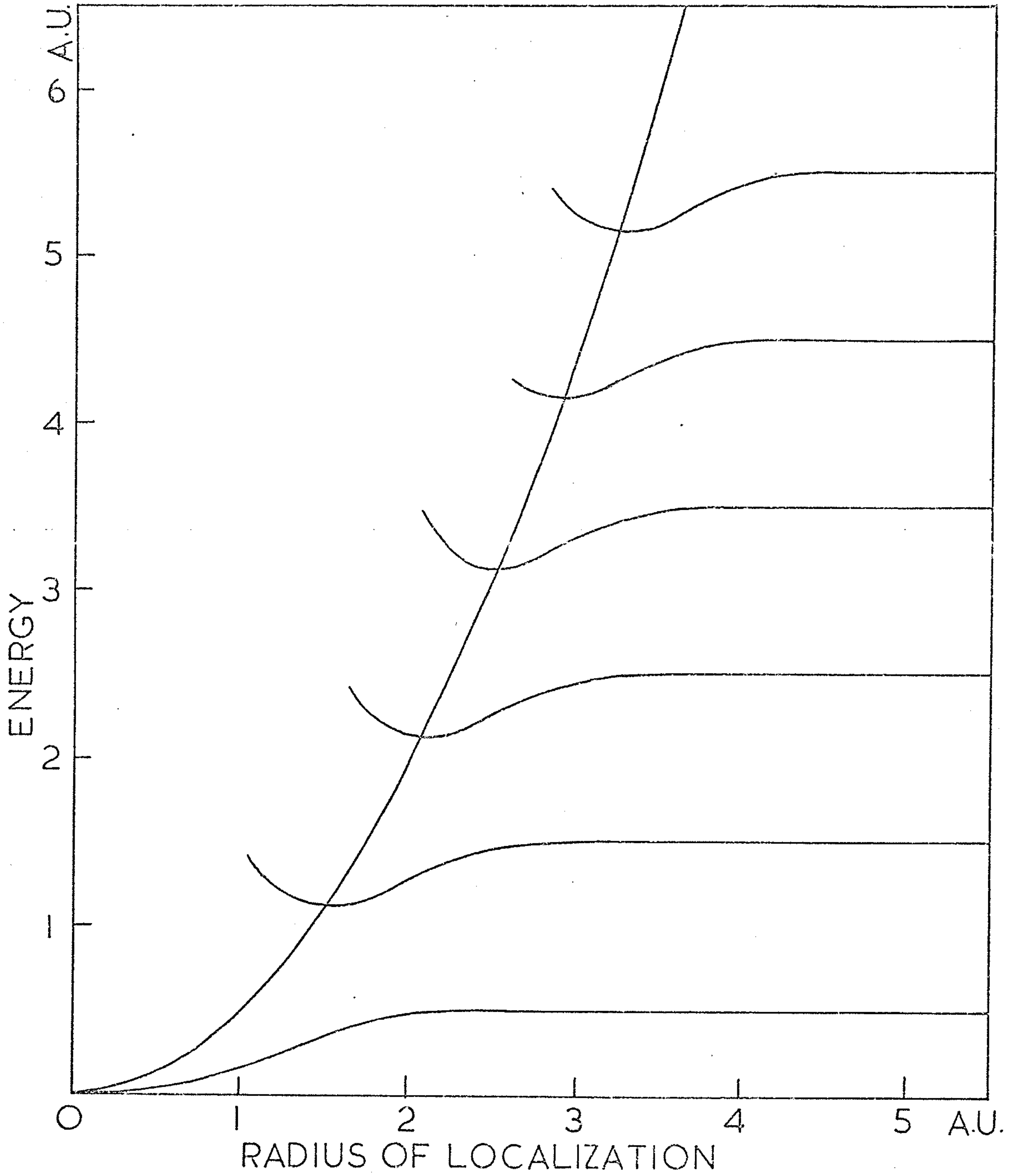


FIGURE 9. Variation of the mean energy of the harmonic oscillator with the radius of localization for the first six states. The mean energy is calculated by using equation 68 with alpha equal to $\frac{1}{2}$pi. The classical limit is drawn in and all parameters are expressed in atomic units.

FIGURE 9

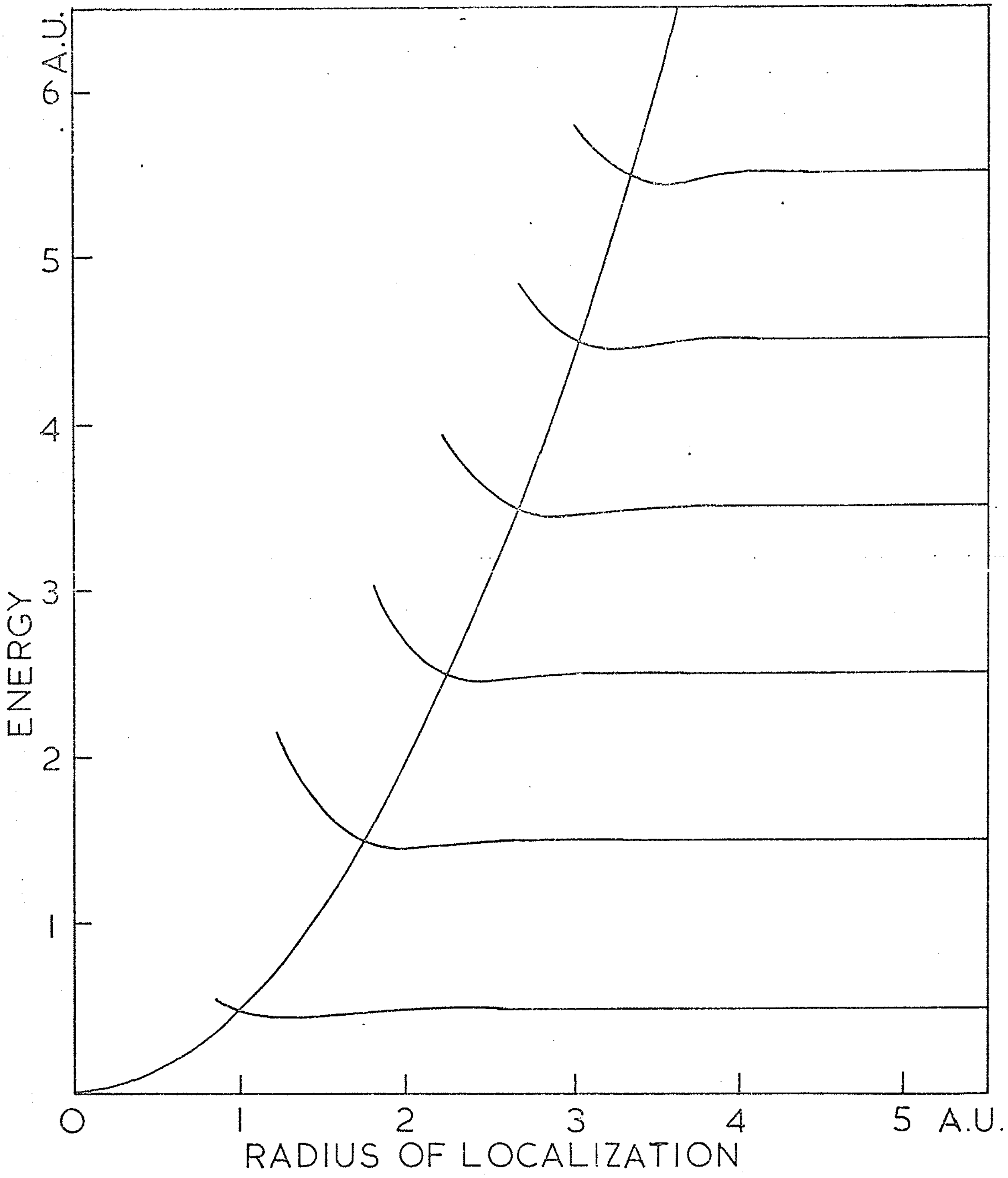


FIGURE 10. Variation of the mean energy of the harmonic oscillator with the radius of localization for the first six states. The mean energy is calculated by using equation 68 with alpha equal to pi for the even states and zero for the odd states. The classical limit is drawn in and all parameters are expressed in atomic units

FIGURE 10

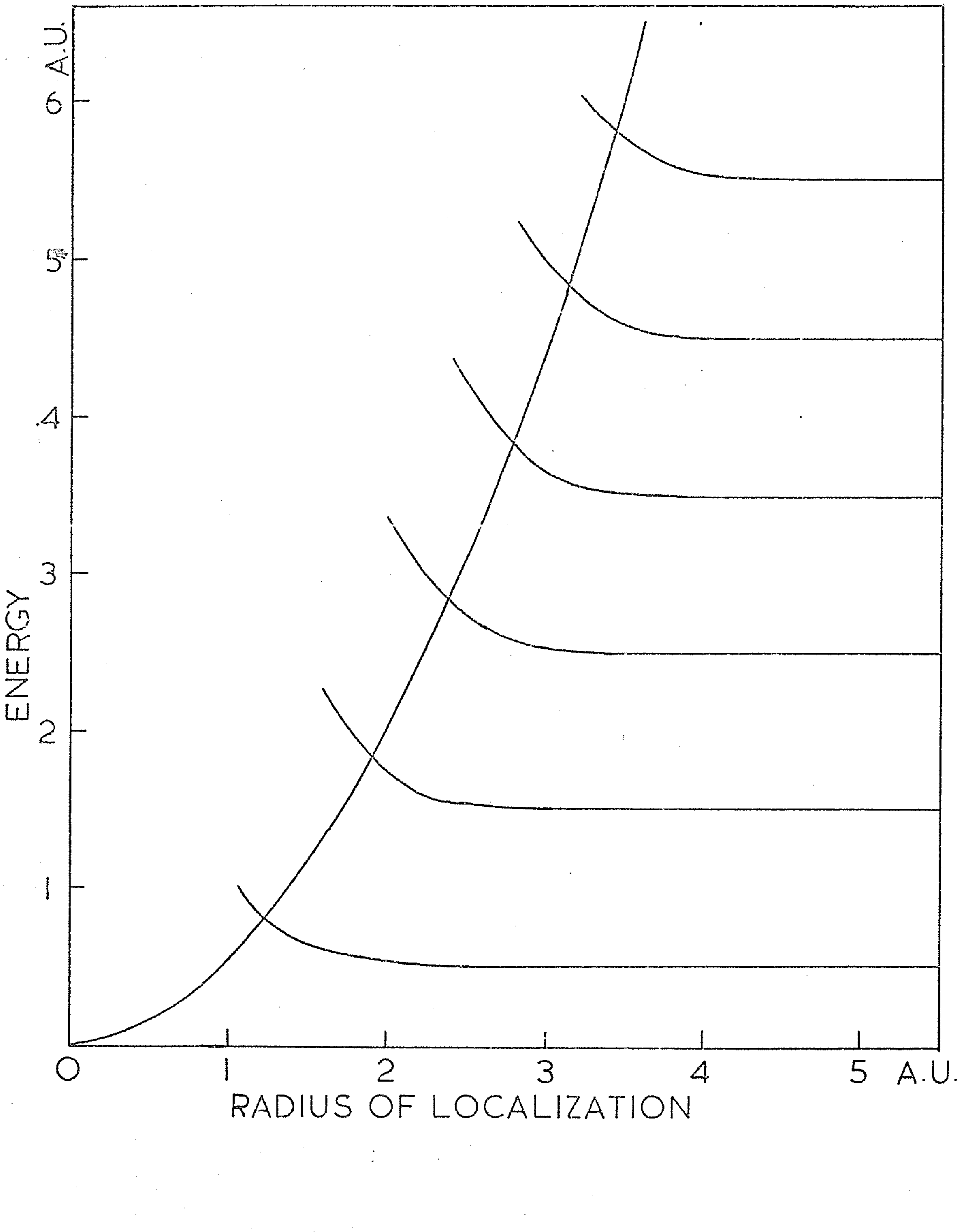


FIGURE 11. Variation of the mean potential (a), kinetic (c) mean energy (b) with alpha for a radius of 1.2964 a.u. for the state 0 of the harmonic oscillator.Equations 65, 67, and 68 are used. The energies are in atomic units and alpha is expressed in radians.

FIGURE II

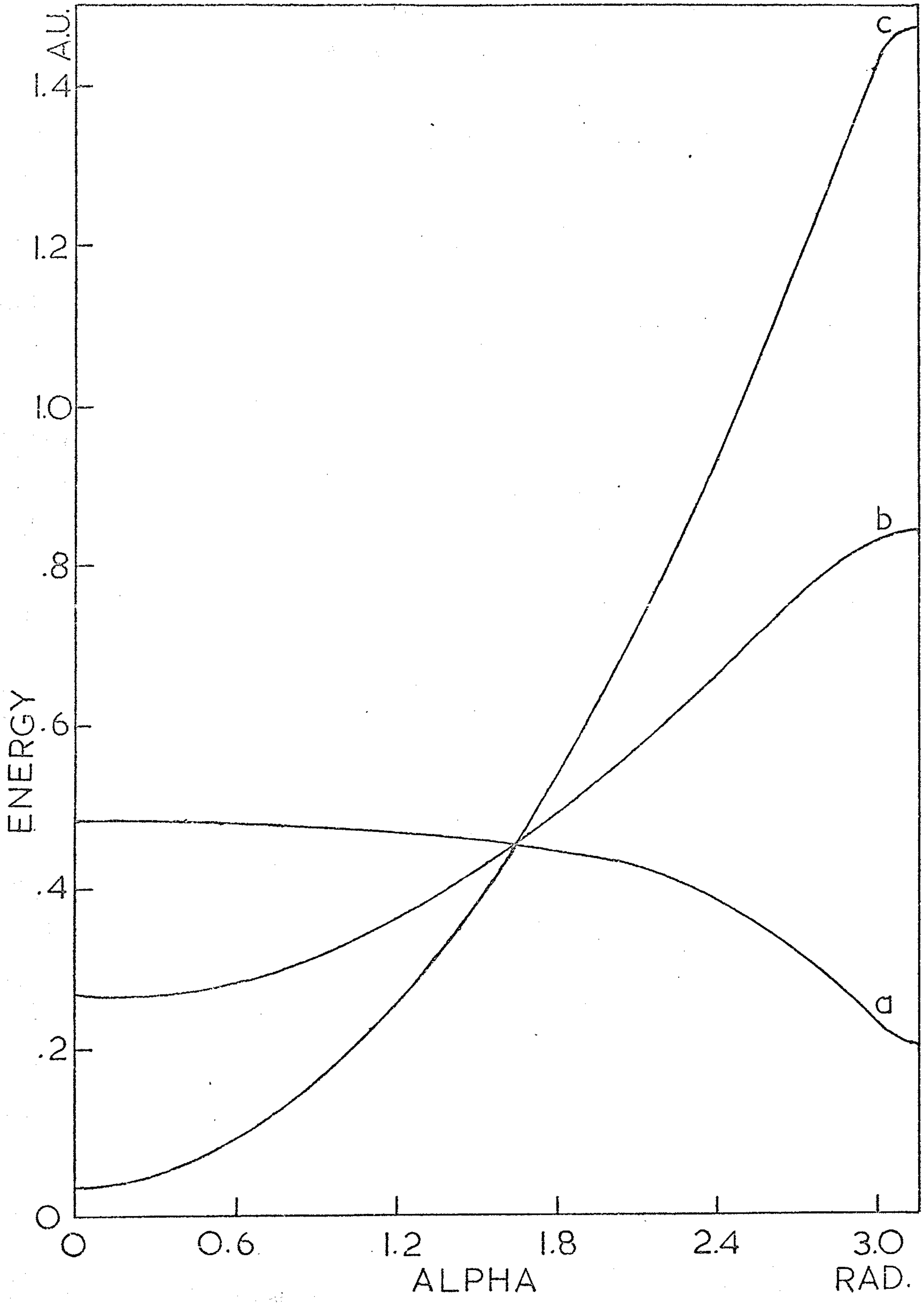


FIGURE 12. Variation in the uncertainty in position (a) and momentum (b) with alpha for a radius of 1.2964 a.u. and state 0 of the harmonic oscillator. The uncertainties are expressed in atomic units and alpha is in radians.

FIGURE 12

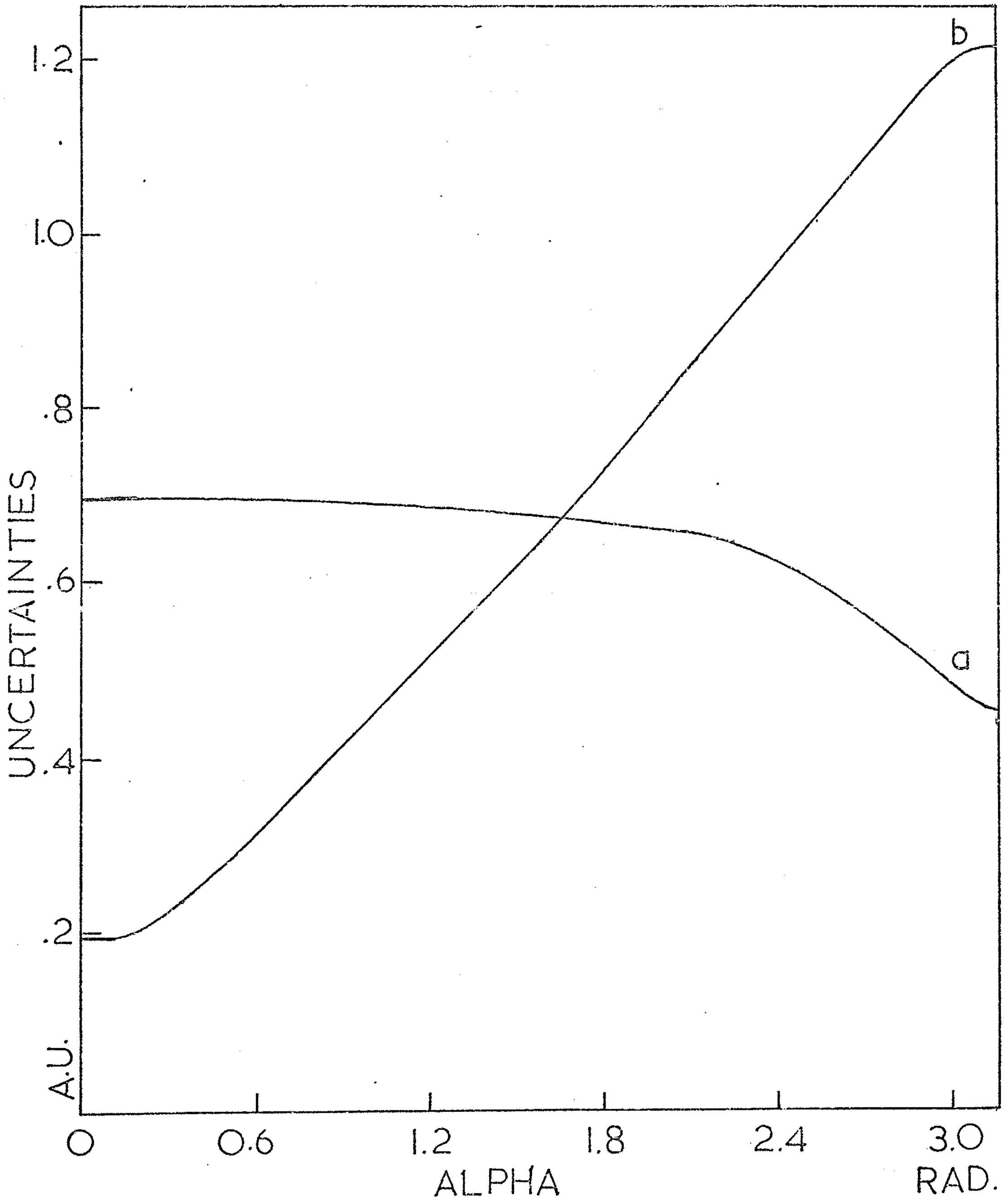


FIGURE 13. Variation of the product of uncertainties with alpha for the ground state and a radius of 1.2964 a.u. The uncertainties are expressed in atomic units and alpha is in radians.

FIGURE 13

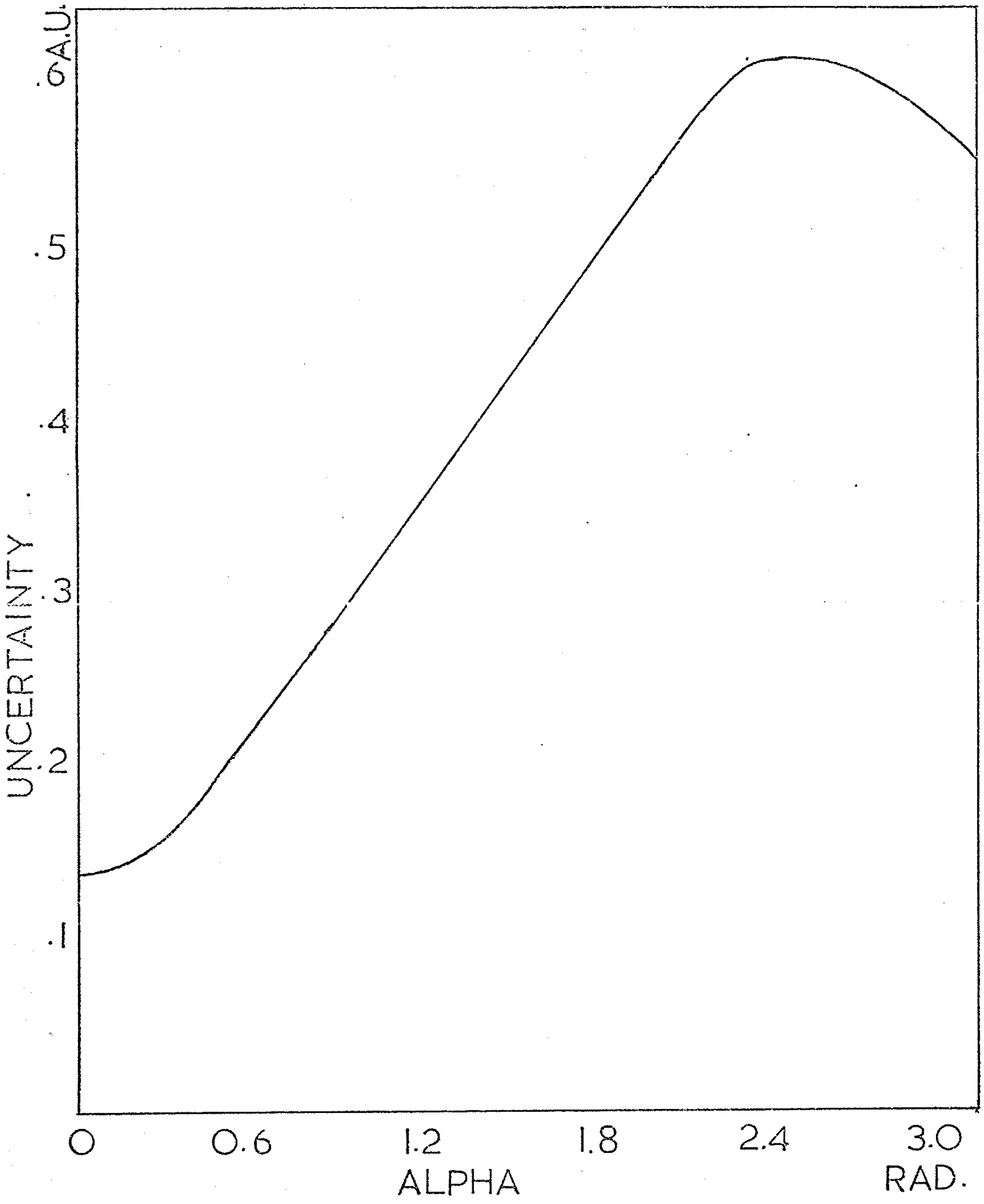


FIGURE 14. Variation of the mean potential and kinetic energy with the radius of localization for the first three states. Alpha is pi for the even states and zero for the odd ones. The mean potential curves are those that go to zero. The classical limit is drawn in and all parameters are given in atomic units.

FIGURE 14

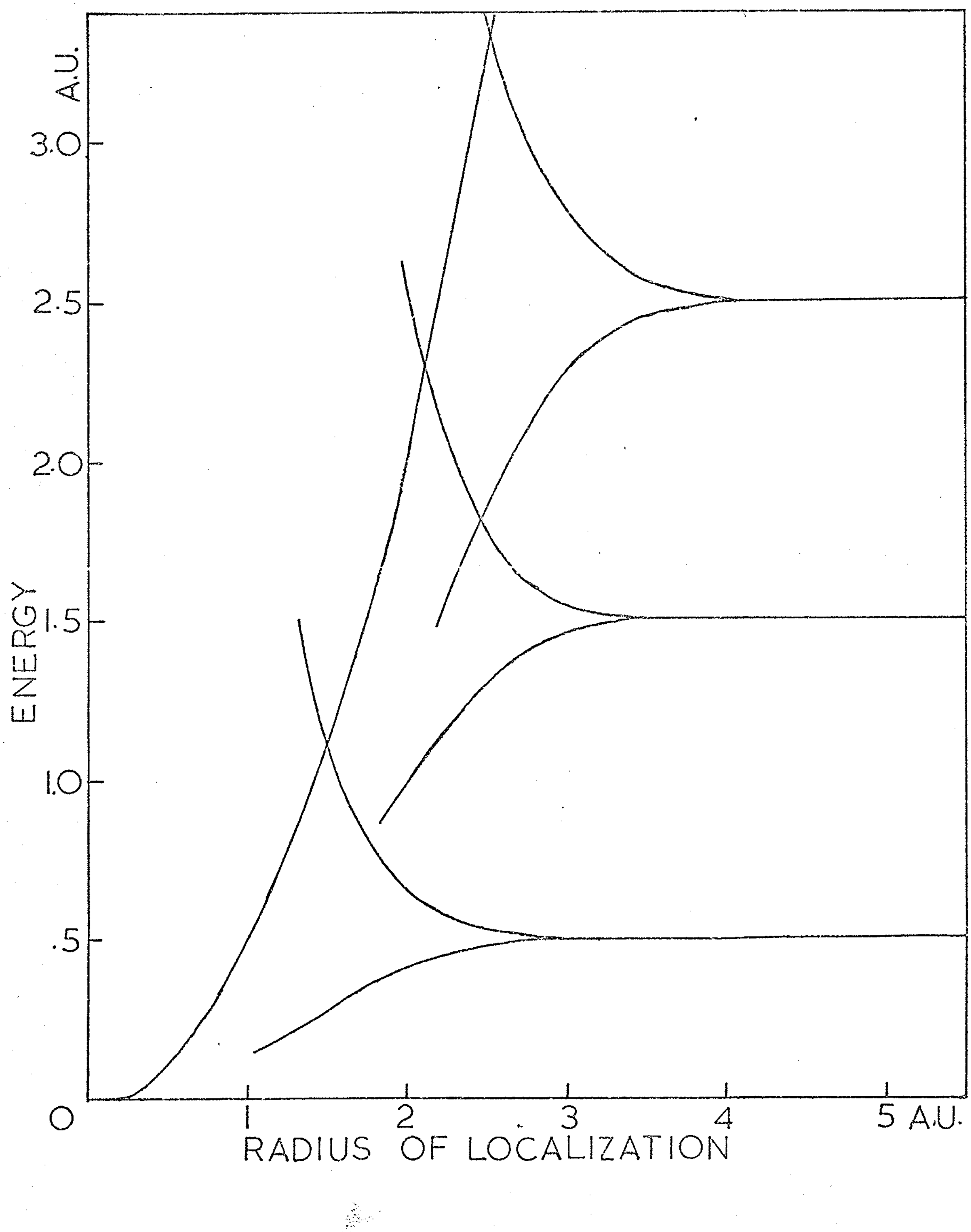


FIGURE 15. Variation of the uncertainty in position (dashed lines) and the product of uncertainties (solid lines) with the radius of localization. Alpha is pi for the even states and zero for the odd ones. All parameters are expressed in atomic units. The first three states are shown.

FIGURE 15

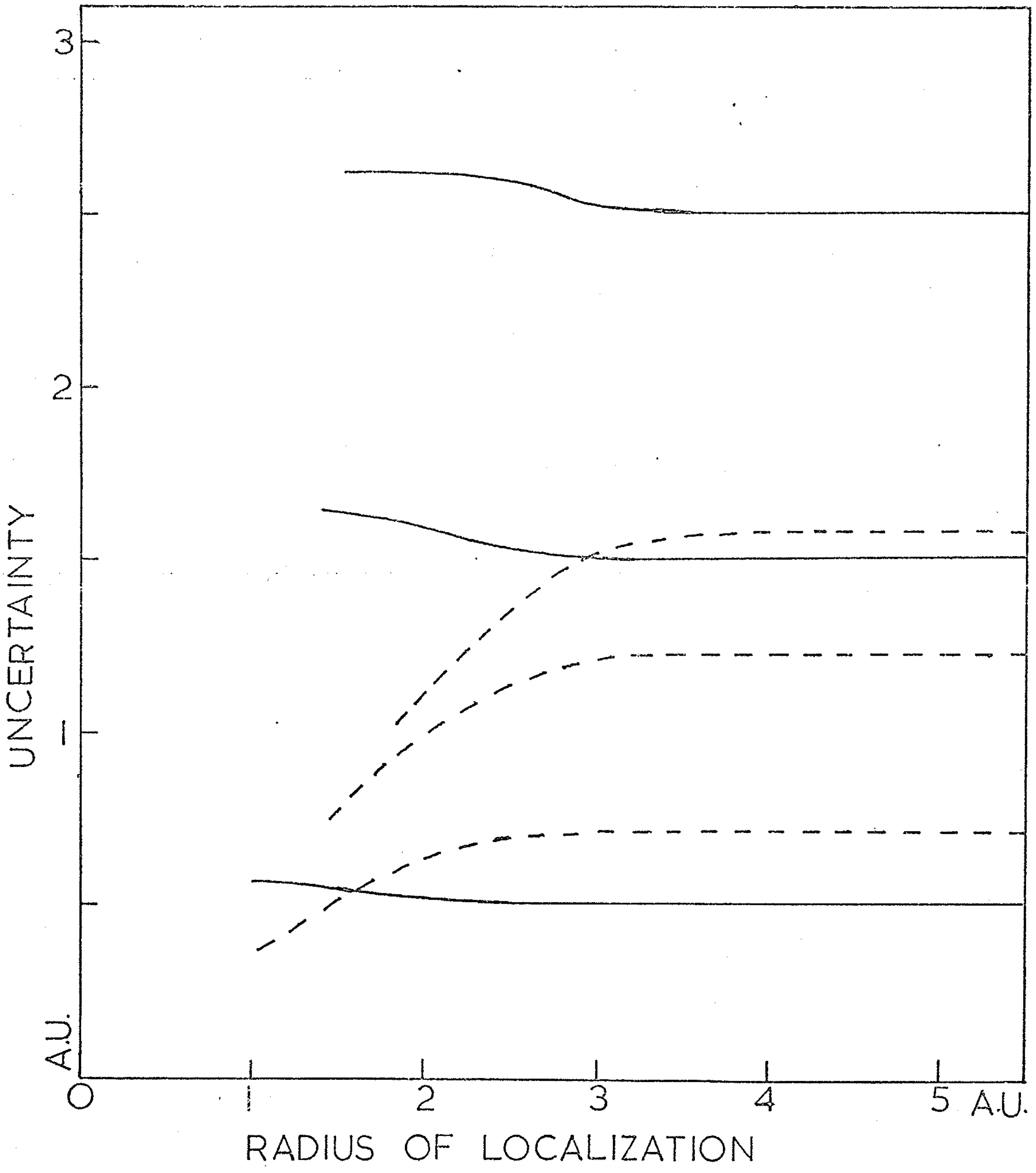


FIGURE 16. Variation of the mean potential (those curves that are concave down) and the mean kinetic energy with the radius of localization. Alpha is zero for the even states and pi for the odd states. All parameters are expressed in atomic units. The classical limit is shown by the vertical lines drawn. The first three states are analyzed.

FIGURE 16

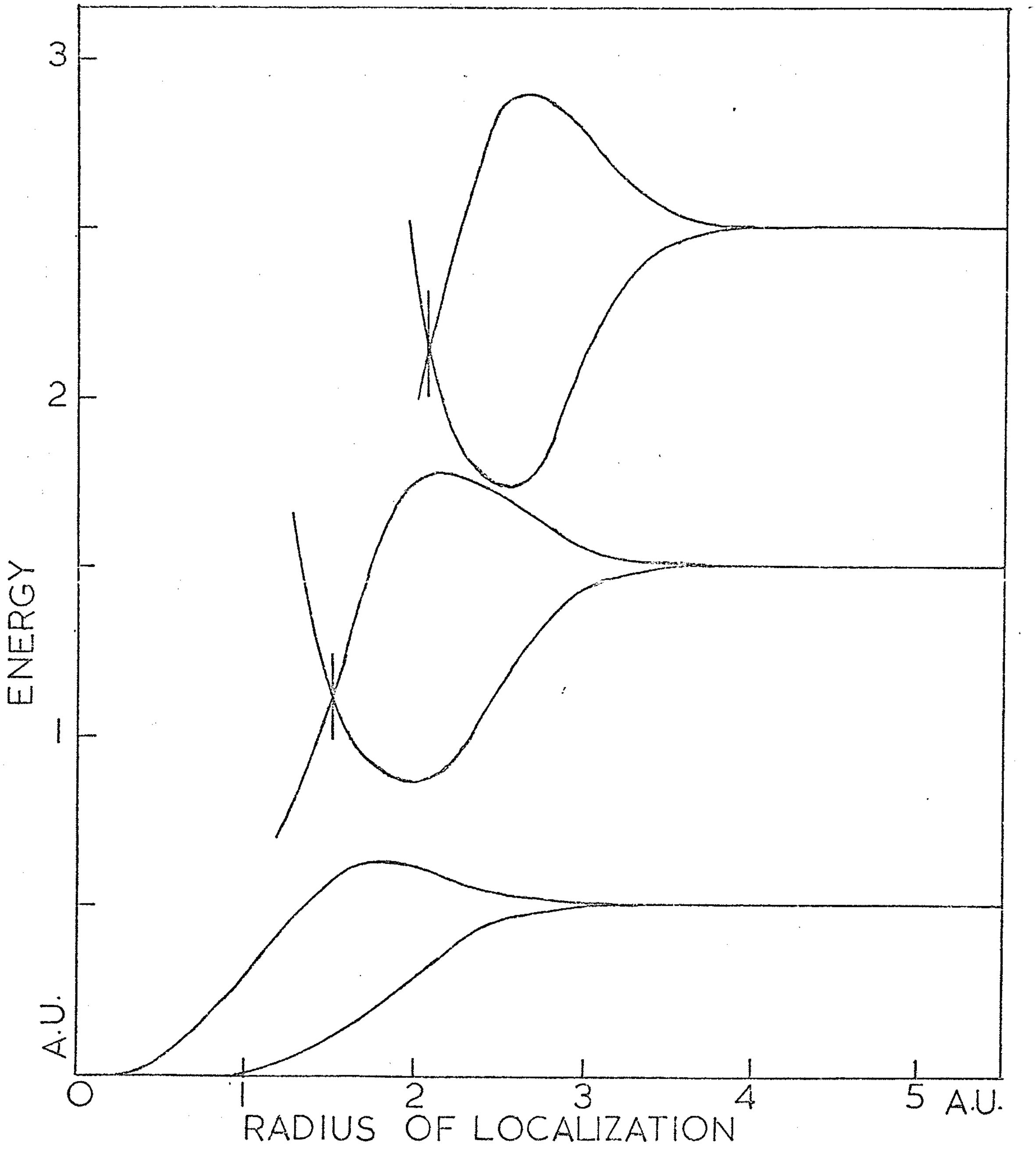


FIGURE 17. Variation of the uncertainty in position (dashed lines) and the product of uncertainties for the first three states with the radius of localization. Alpha is zero for the even states and pi for the odd ones. All parameters are expressed in atomic units.

FIGURE 17

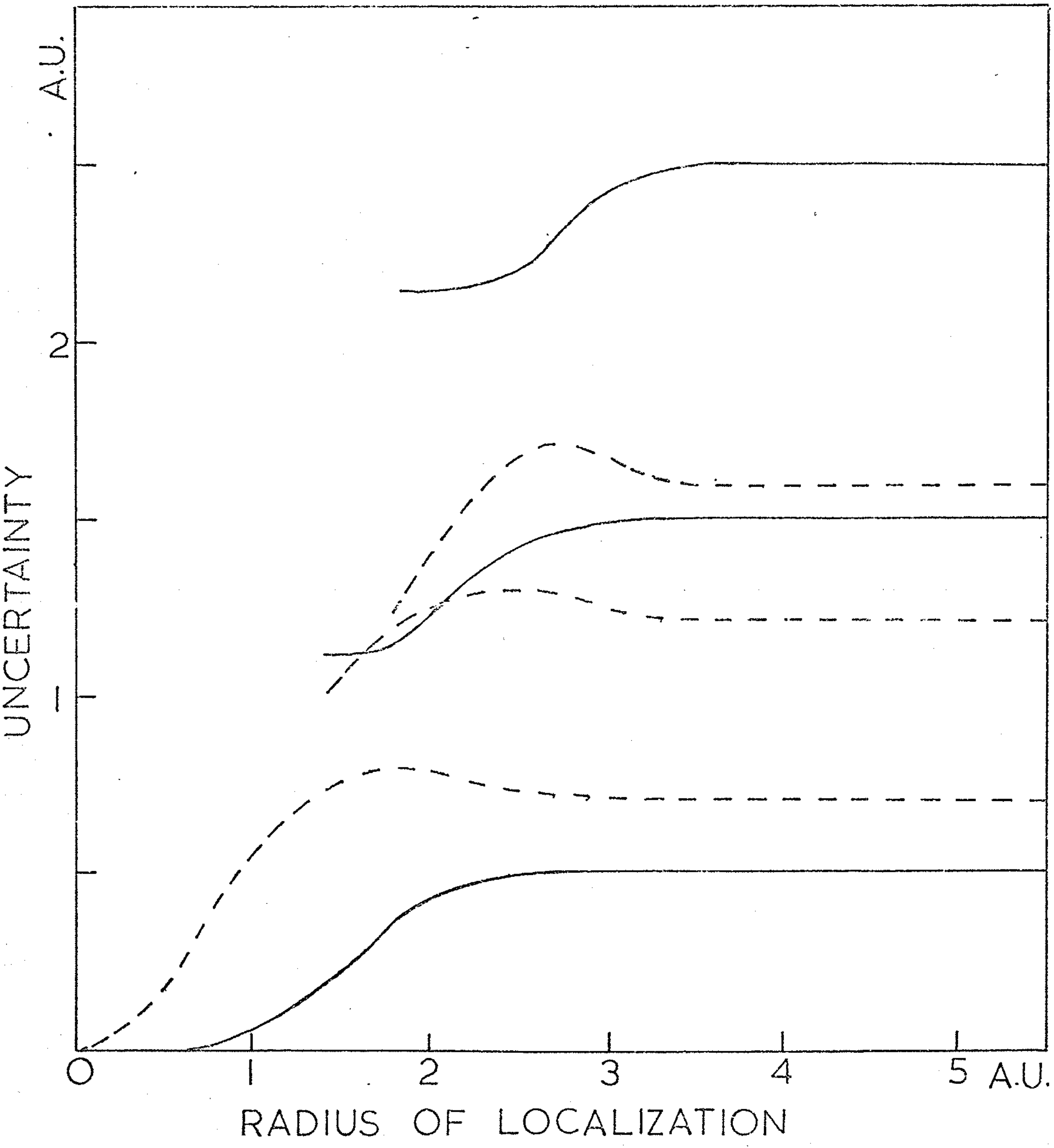


FIGURE 18 Variation of the mean potential (those curves that are concave down) and the mean kinetic energy for the first three states with the radius of localization. Alpha is $\frac{1}{2}$pi. All parameters are expressed in atomic units

FIGURE 18

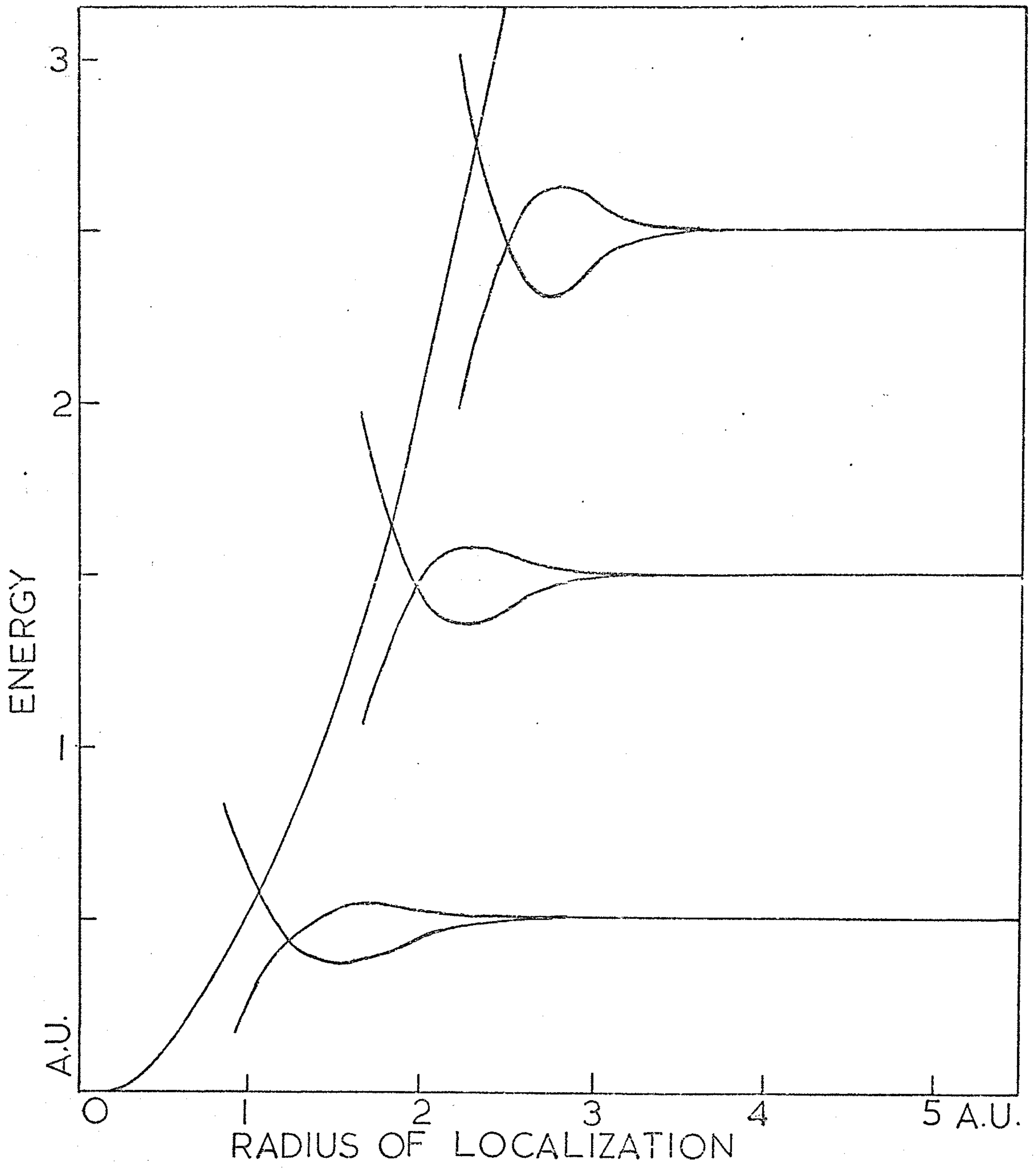


FIGURE 19. Variation of the uncertainty in position (dashed lines) and the product of uncertainties for the first three states with the radius of localization. All parameters are in atomic units, and alpha has a value of $\frac{1}{2}$pi.

FIGURE 19

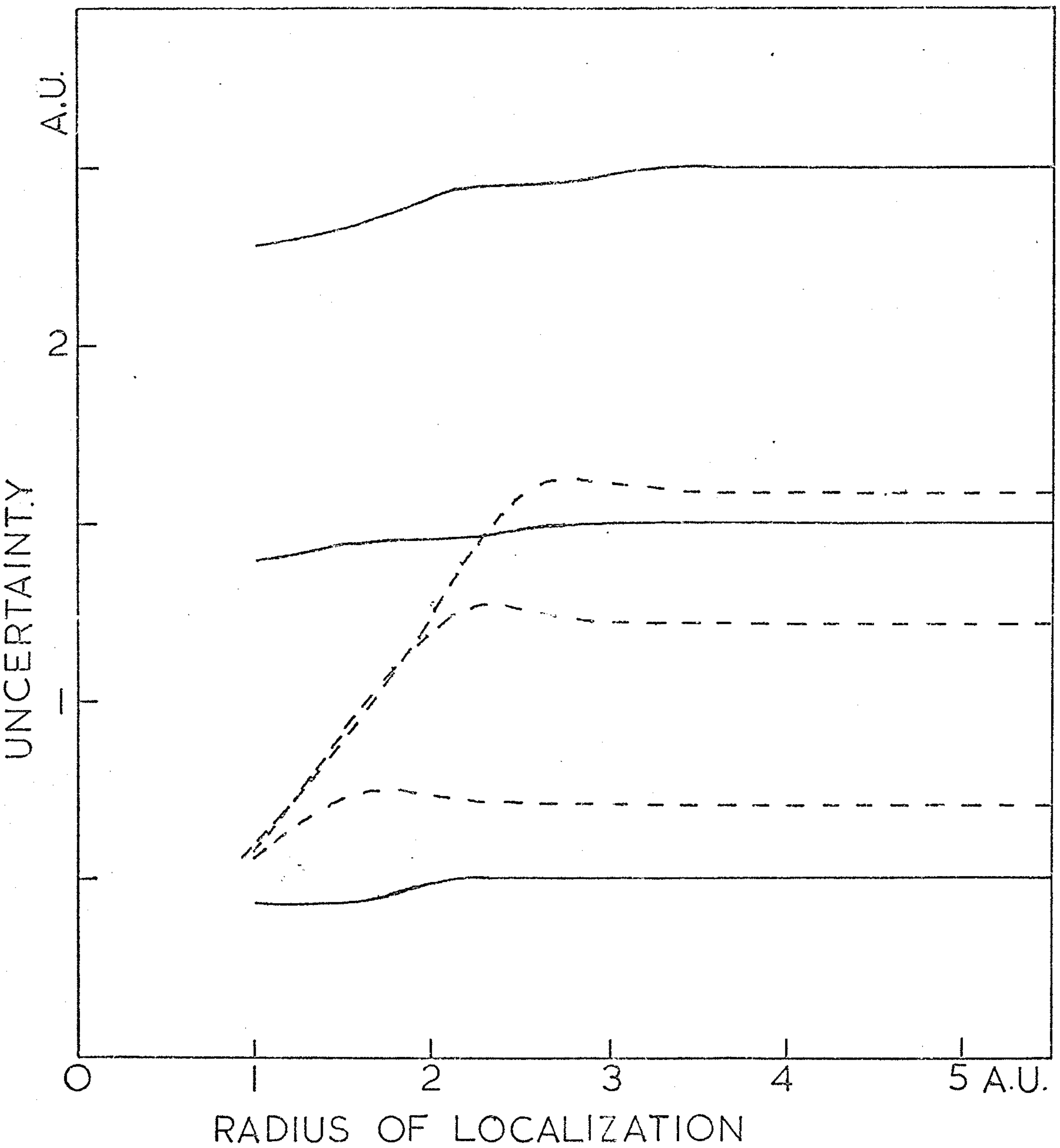


FIGURE 20. Plot of the distribution for the first excited state function classically localized. Alpha is pi for the upper graph and $\frac{1}{2}$pi for the lower one. Equation 80 is used and all parameters are expressed in atomic units.

FIGURE 20

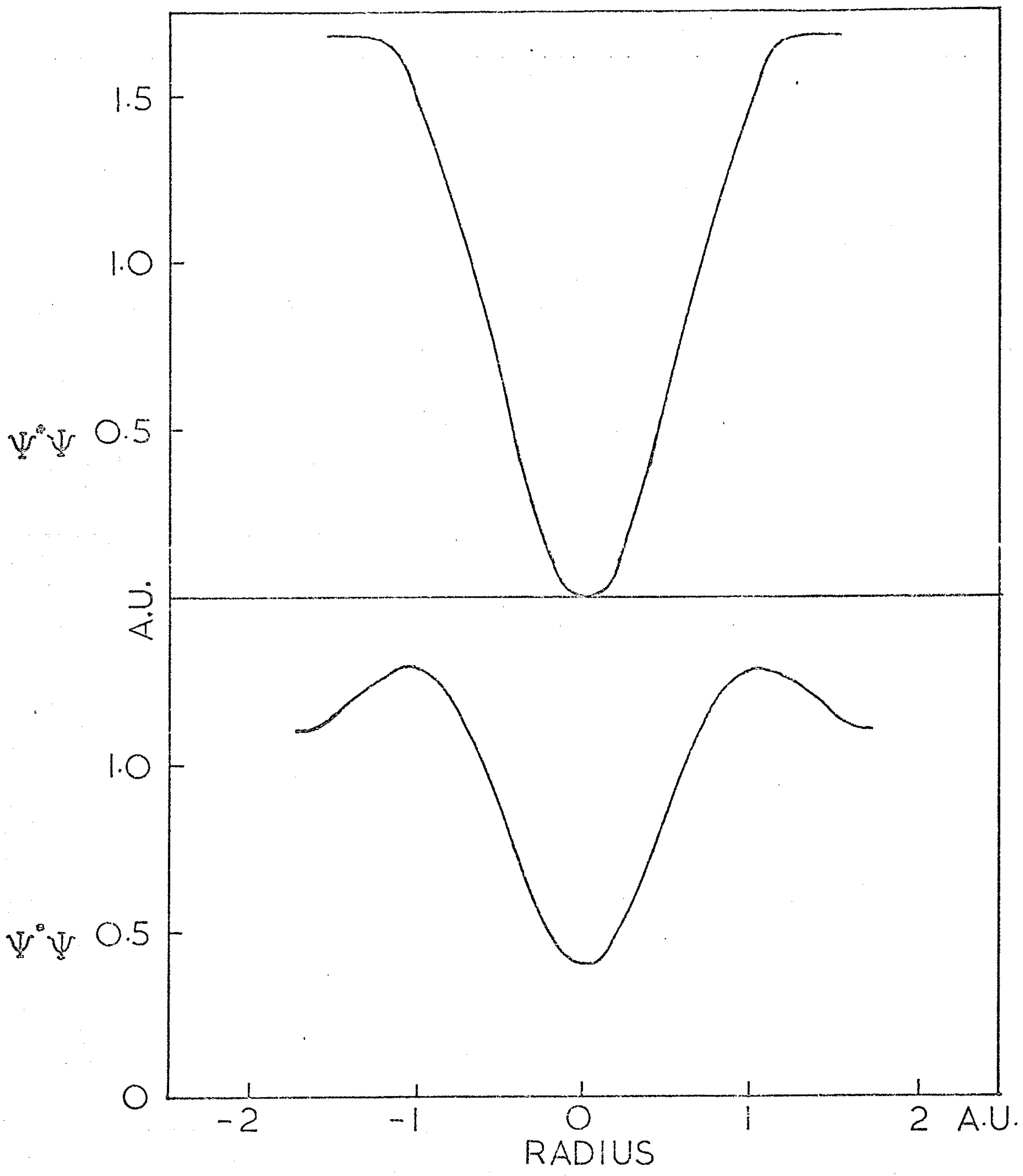
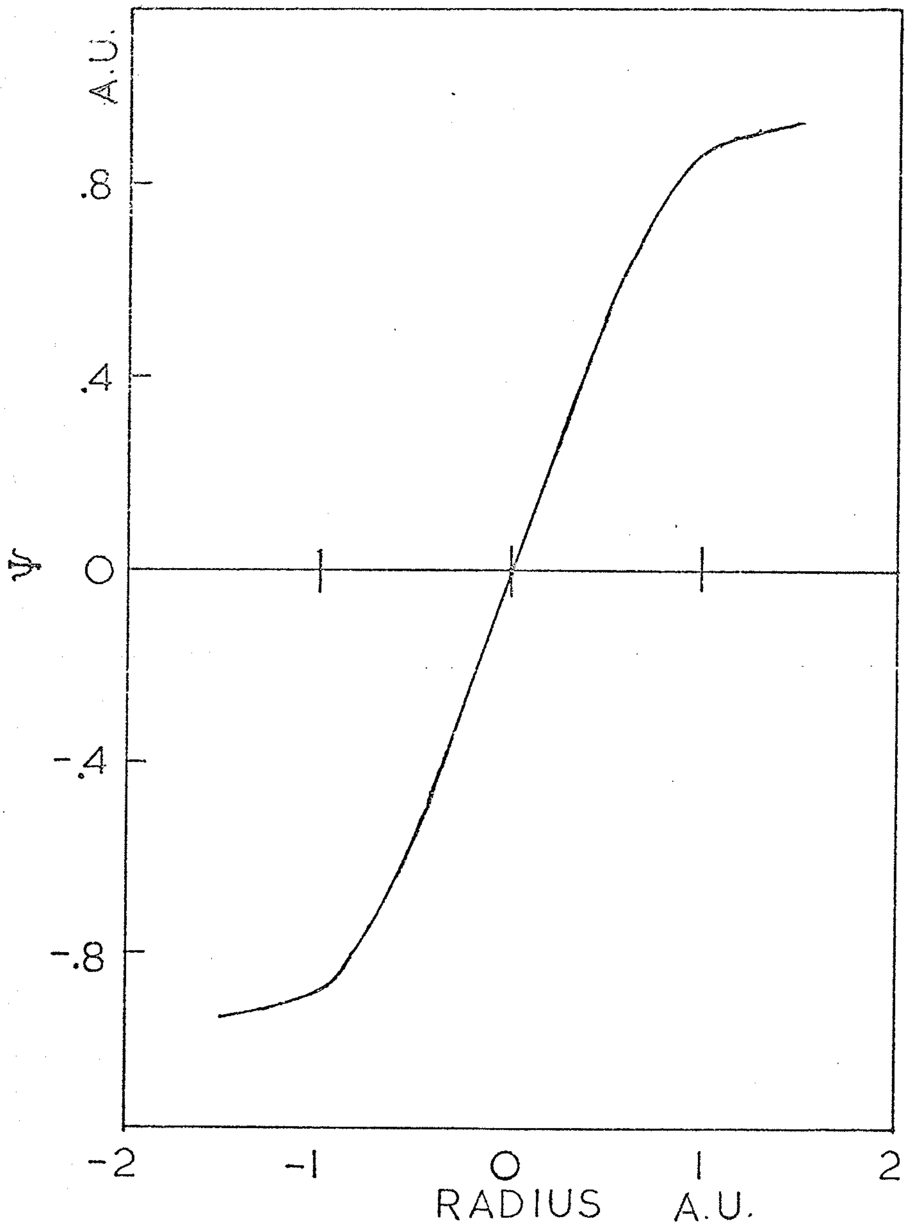


FIGURE 21. Plot of the first excited state with alpha equal to pi. Equation 75 is used and all parameters are expressed in atomic units.

FIGURE 21



DISCUSSION OF RESULTS

Basic calculations indicate that the Jauch and Piron (25) concept of localizability (i.e. being contained in a certain region of space) is as valid as the infinite domain formulation. This is established by figures 1,3,7, etc. that show the energy spectrum to be constantly spaced until the classical domain is reached. This formulation, using localizability as a basic feature, is a more general one with the infinite domain being one of many special cases. The finite difference and the fourier analysis approaches represent a rigorous approach to the problem of localization and are equally successful. The finite difference method becomes more versatile as the system becomes more complex and requires complicated functions. It overcomes difficulties ocurring in finding the correct functions and the integrals that involve them. The Heaviside function approach is basically no more satisfying conceptually than the infinite domain formulation since the distribution approach requires the existence of wave functions defined on the infinite domain. This is not present in the other methods of localization and they represent an alternative point of view that Schrodinger discarded.

In a low energy collision between a hydrogen atom and a proton, using wave functions defined on an infinite domain, the electron is regarded as being shared equally by both atomic centres. With localization theory the electron is bound to one atomic centre until a hydrogen molecule ion is formed. Polarization of the electron is basically the only phenomenon occurring until the two domains overlap. In isolating the two systems the Schrodinger equations used to describe the process can be simplified without resorting to some ad hoc approximation as neglecting overlap integrals. This is shown mathematically by co-workers (41) in the application of a of a localized hydrogen atom to collision processes.

Although the various approaches are successful in predicting an energy spectrum that agrees with one special case previously accepted (this is basically the only criterion of success as the model is only theoretical) several difficulties still exist to be overcome. Some estimation of the uncertainty in energy is required to indicate how precise the energy remains as the system is localized. The wave packet approach offers some approximate method for this, but the complexity of distributions makes its evaluation difficult. In the extension to a hydrogen atom (41) the problem is overcome as a simple step function is employed. Quantum tunneling, easily explained with wave functions defined on an infinite domain, needs some mechanism for occurring in the local representation when the domains of the two systems are not overlapping. This however is not a serious drawback.

The extension of these methods to more complicated systems is not easily accomplished. For the hydrogen atom, the distribution theory approach becomes workable as the simple step function is used with polynominals other than the hermite ones. A three dimensional analogue to the oscillator in a box, or the bounded operator has been accomplished, but only for a constant potential V_0 (40). In the extension to a hydrogen atom, i.e. a varying potential, completeness of the set of functions used to describe the energy appears to be a major problem. The finite difference method, which uses no function set, provides the best means for localizing the hydrogen atom by solving the differential equation on a bounded interval.

The concept of local states, originally researched to simplify collision calculations, also follows a mainstream of physics in questioning the mathematical formalism of quantum mechanics (42). By creating local states, the Einstein, Podolsky, Rosen paradox does not exist as mutually distant systems would then become independent of each other. This problem had been introduced into quantum mechanics to question the concept of causality that had been formulated in the Copenhagen interpretation of the wave function. It endeavoured to illustrate that a deeper theory was required to explain the action of an electron and not a series of experiments predicting its probable behaviour. This has since affected our concept of the measurement process and many theories (mainly hidden variable ones) have been expounded in order to create a causal explanation of phenonema. The following of this present line of thought and in particular the relation of local states to these theories could lead to a more inclusive explanation of fact.

DEFINITIONS USED IN WAVE PACKET APPROACH

1. Step Function

$$S(x-x_o) = 1 \quad x \leq x_o$$
$$= 0 \quad x > x_o$$

2. Dirac Delta Function

$$\delta(x-x_o) = \frac{d}{dx} S(x-x_o)$$

$$\delta(x-x_o) = 0 \quad x \neq 0$$
$$= \infty \quad x = 0$$
$$\int_{-\infty}^{\infty} \delta(x)dx = 1$$

3. Heaviside Step Function

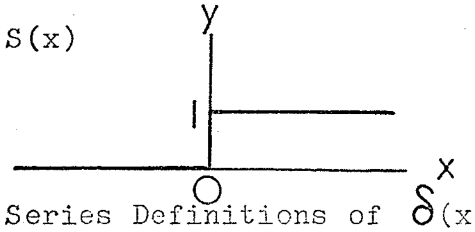
$$\theta(a,b) = 1 \quad a \leq x \leq b$$

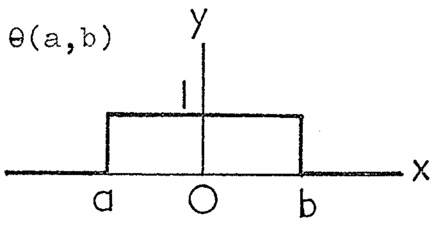
$$= 0 \quad x > a,\ x < b$$

In terms of $S(x-x_o)$, $\theta(a,b)$ can be written:

$S(x+ a)[1 - S(x-b)]$

Pictorally these are:





Series Definitions of $\delta(x)$, $S(x)$

$\delta(x)$

$$\phi_n(x) = \lim_{n\to\infty} \frac{n}{\sqrt{\pi}} e^{-n^2x^2}$$

$S(x)$

$$\Phi_n(x) = \lim_{n\to\infty} \int_{-\infty}^{x} \phi_n(\xi)d\xi$$

$\phi_n(x)$ can also be put in the form:

$$\frac{n}{\pi}\,\frac{1}{1+n^2x^2} \quad ; \quad \frac{1}{n\pi}\,\frac{\sin^2(nx)}{x^2}$$

Formal definitions used in Distribution Theory can be found in references 34,35, and in particular, in Butkov,E., Mathematical Physics, Addison-Wesley, 1968, p.221-255.

The Hermite Polynomials used in this thesis are defined by the equation:

$$H_n(x) = (-)^n e^{x^2}\left[\frac{d^n}{dx^n}e^{-x^2}\right] \qquad n = 0,1,2,3,\ldots..$$

Some pertinent recursion formulae are:

1. $2x\,H_n(x) = H_{n+1}(x) + 2n\,H_{n-1}(x)$
2. $H_n(x) = \sum_{k=0}^{[n/2]} \frac{(-)^k n!}{k!(n-2k)!}(2x)^{n-2k}$ for $n > 1$

$[n/2]$ indicates $n/2$ for even n and $(n-1)/2$ for odd n

Special integration formulae pertaining to the Hermite Polynomials can be found in: Bateman Manuscript Project, California Institute of Technology, McGraw-Hill, 1953-55. Vol. 1-4.

INTEGRAL EVALUATIONS FOR THE OSCILLATOR IN A BOX

TRIGONOMETRIC FUNCTIONS USED

$$\cos^2(x) = \tfrac{1}{2}[1 + \cos(2x)] \tag{b-1}$$

$$\sin^2(x) = \tfrac{1}{2}[1 - \cos(2x)] \tag{b-2}$$

$$\cos(ax).\cos(bx) = \tfrac{1}{2}[\cos\ (a+b)x + \cos\ (a-b)x\ ] \tag{b-3}$$

$$\sin\ (ax).\sin(bx) = \tfrac{1}{2}[\cos\ (a+b)x - \cos\ (a-b)x\ ] \tag{b-4}$$

STANDARD INTEGRAL USED

$$\int_{-b}^{b} x^2\cos(ax)dx = 4b\ \frac{\cos(ab)}{a^2} + \frac{2a^2b^2 - 2}{a^3}\ \sin(ab) \tag{b-5}$$

This is integral 329 in the Handbook of Chemistry and Physics - Chemical Rubber Company, 49th edition.

NORMALIZATION

Even States

$$I = \sum_{m,n} c_n c_m \int_{-a}^{a} \cos(m\pi x/2a)\ \cos(n\pi x/2a)\ dx \tag{b-6}$$

For $m = n$

$$I = \sum_{n} c_n^2 \int_{-a}^{a} \cos^2(n\pi x/2a)\ dx \tag{b-7}$$

$$= \sum_{n} c_n^2 \int_{-a}^{a} \tfrac{1}{2}[1 + \cos(n\pi x/a)]\,dx \tag{b-8}$$

$$= \sum_{n} c_n^2\ \tfrac{1}{2}[x + \frac{a}{n\pi}\ \sin(n\pi x/a)\ ] \tag{b-9}$$

$$= a \sum_{n} c_n^2 \tag{b-10}$$

The sine of $n.\pi$ is zero

For $m \neq n$

$$I = \sum_{m \neq n} c_n c_m \int_{-a}^{a} \tfrac{1}{2}(\cos[\ (m+n)\pi x/2a] + \cos\ [(m-n)\pi\ x/2a])dx \tag{b-11}$$

$$I \sim \sin\,(m+n)\pi/2 - \sin\,(m-n)\pi/2 = 0 \qquad \text{b-12}$$

m,n are always odd; the sum or difference of two odd numbers is even. Therefore the sine functions of b-12 are zero.

Odd States

$$I = \sum_{m,n} c_n c_m \int_{-a}^{a} \sin(n\pi x/a)\,\sin(m\pi x/a)dx \qquad \text{b-13}$$

For $m = n$

$$I = \sum_{n} c_n^2 \int_{-a}^{a} \tfrac{1}{2}[1 - \cos(2n\pi x/a)]\,dx \qquad \text{b-14}$$

$$= \sum_{n} c_n^2 \left[a - \frac{a}{n\pi}\sin(2n\pi)\right] \qquad \text{b-15}$$

$$= a\sum_{n} c_n^2 \qquad \text{b-16}$$

For $m \neq n$

$$I = \sum_{m,n} c_n c_m \int_{-a}^{a} \tfrac{1}{2}[\cos[(m-n)\pi x/a] - \cos[(m+n)\pi x/a]]dx \qquad \text{b-17}$$

$$\sim \sin[(m-n)\pi] - \sin[(m+n)\pi] = 0 \qquad \text{b-18}$$

KINETIC ENERGY

Even States

$$\langle p^2 \rangle = \sum_{m,n} c_n c_m \int_{-a}^{a} \cos(n\pi x/2a).\frac{-d^2}{dx^2}\cos(m\pi x/2a)\,dx \qquad \text{b-19}$$

$$= \sum_{m,n} c_n c_m \frac{m\pi^2}{2a}\int_{-a}^{a} \cos(n\pi x/2a)\,\cos(m\pi x/2a)\,dx \qquad \text{b-20}$$

$$= \frac{\pi^2}{4a}\sum_{m} m^2 c_m^2 \qquad \text{b-21}$$

Odd States

$$\langle p^2 \rangle = \sum_{m,n} c_n c_m \int_{-a}^{a} \sin(n\pi x/a).\frac{-d^2}{dx^2}\sin(m\pi x/a)\,dx \qquad \text{b-22}$$

$$\langle p^2 \rangle = \frac{\pi^2}{a} \sum_n n^2 c_n^2 \tag{b-23}$$

POTENTIAL ENERGY

Even States

$$\langle x^2 \rangle = \sum_{m,n} c_n c_m \int_{-a}^{a} x^2 \cos(n\pi x/2a)\, \cos(m\pi x/2a)\, dx \tag{b-24}$$

For $m = n$

$$\langle x^2 \rangle = \sum_n c_n^2 \int_{-a}^{a} x^2 \cos^2(n\pi x/2a)\, dx \tag{b-25}$$

$$= \sum_n c_n^2 \int_{-a}^{a} x^2 \tfrac{1}{2}[1+\cos(n\pi x/a)]\, dx \tag{b-26}$$

$$= \sum_n c_n^2 \left[\frac{a^3}{3} + \frac{2a^3 \cos(n\pi)}{(n\pi)^2}\right] \tag{b-27}$$

The sine of $n.\pi$ is zero and can be dropped from the integral expression of b-5.

For $m \neq n$

$$\langle x^2 \rangle = \tfrac{1}{2} \sum_{m\neq n} c_n c_m \int_{-a}^{a} x^2 [\cos[(m+n)\pi x/2a] + \cos[(m-n)\pi x/2a]] dx \tag{b-28}$$

$$= 2 \sum_{m\neq n} c_n c_m\, a^3 \left[\frac{\cos[(m+n)\pi/2]}{[(m+n)\pi/2]^2} + \frac{\cos[(m-n)\pi/2]}{[(m-n)\pi/2]^2}\right] \tag{b-29}$$

The sine term again cancels itself.

Odd States

$$\langle x^2 \rangle = \sum_{m,n} c_n c_m \int_{-a}^{a} x^2 \sin(n\pi x/a)\, \sin(m\pi x/a)\, dx \tag{b-30}$$

For $m = n$

$$\langle x^2 \rangle = \tfrac{1}{2} \sum_n c_n^2 \int_{-a}^{a} x^2 [1-\cos(2n\pi x/a)]\, dx \tag{b-31}$$

$$\langle x^2 \rangle = \sum_n c_n^2 \left[\frac{a^3}{3} - 2a \, \frac{\cos(2n\pi)}{(2n\pi/a)^2} \right] \qquad \text{b-32}$$

$$= \sum_n c_n^2 \left[\frac{a^3}{3} - \frac{a^3}{2(n\pi)^2} \right] \qquad \text{b-33}$$

As n is always an integer, 2n is always an even integer whose cosine is one.

For $m \neq n$

$$\langle x^2 \rangle = \tfrac{1}{2} \sum_{m \neq n} c_n c_m \int_{-a}^{a} x^2 [\cos[(m-n)\pi x/a] - \cos[(m+n)\pi x/a]] \, dx \qquad \text{b-34}$$

$$= 2a^3 \sum_{m \neq n} c_n c_m \left[\frac{\cos[(m-n)\pi]}{[(m-n)\pi]^2} - \frac{\cos[(m+n)\pi]}{[(m+n)\pi]^2} \right] \qquad \text{b-35}$$

The sine terms are again zero.

For the odd states the energy matrix is:

$$\frac{\pi^2}{2a^2} \sum_n c_n^2 n^2 + \sum_n c_n^2 a^2 \left[\frac{1}{6} + \frac{1}{4(n\pi)^2} \right] + a^2 \sum_{m \neq n} c_n c_m \left[\frac{\cos[(m+n)\pi]}{[(m+n)\pi]^2} + \frac{\cos[(m-n)\pi]}{[(m-n)\pi]^2} \right] = E \sum_n c_n^2 \qquad \text{b-36}$$

Differentiating with respect to c_k

$$c_k \left[\frac{\pi^2 k^2}{a^2} + a^2 \left(\frac{1}{3} + \frac{1}{2(n\pi)^2} \right) \right] + a^2 \left\{ \sum_n c_n \left[\frac{\cos[(k-n)\pi]}{[(k-n)\pi]^2} + \frac{\cos[(k+n)\pi]}{[(k+n)\pi]^2} \right] + \sum_m c_m \left[\frac{\cos[(k-m)\pi]}{[(k-m)\pi]^2} + \frac{\cos[(k+m)\pi]}{[(k+m)\pi]^2} \right] \right\} = 2Ec_k \qquad \text{b-37}$$

Since m and n are dummy variables they can be combined and for each k there is a simultaneous set of linear equations given by:

$$\sum c_n \left\{ \frac{\pi^2 k^2}{2a^2} + a^2 \left[\frac{1}{6} + \frac{1}{4(k\pi)^2} \right] - E\,\delta_{kn} + a^2 \left[\frac{\cos[(k+n)\pi]}{[(k+n)\pi]^2} + \frac{\cos[(k-n)\pi]}{[(k-n)\pi]^2} \right] (1-\delta_{kn}) \right\} = 0 \qquad \text{b-38}$$

INTEGRAL EVALUATIONS FOR THE BOUNDED OPERATOR

NORMALIZATION

$$I = \frac{1}{2a}\int_{-a}^{a} e^{-i\pi(\alpha/2\pi+k)x/a}\, e^{i\pi(\alpha/2\pi+k)x/a}\,dx \qquad \text{c-1}$$

$$= \frac{1}{2a}\int_{-a}^{a} e^{-i\pi(k-1)x/a}\,dx \qquad \text{c-2}$$

For $k = 1$

$$I = \frac{1}{2a}\int_{-a}^{a} 1dx = \frac{1}{2a}\, x\Big|_{-a}^{a} = 1 \qquad \text{c-3}$$

For $k \neq 1$

$$I = \frac{1}{2a}\int_{-a}^{a} e^{-i\pi(k-1)x/a}\,dx \qquad \text{c-2}$$

$$I = \frac{1}{2a}\cdot\frac{-a}{i\pi(k-1)}\cdot e^{-i\pi(k-1)x/a}\Big|_{-a}^{a} \qquad \text{c-4}$$

$$= \frac{-1}{2i\pi(k-1)}\left[e^{-i\pi(k-1)} - e^{i\pi(k-1)}\right] \qquad \text{c-5}$$

Using the identity:

$$e^{ix} = \cos(x) + i\sin(x) \qquad \text{c-6}$$

$$e^{-ix} = \cos(x) - i\sin(x) \qquad \text{c-7}$$

$$I = \frac{-1}{2i\pi(k-1)}\cdot\Big[\cos[\pi(k-1)] - i\sin[\pi(k-1)] - \cos[\pi(k-1)] - i\sin[\pi(k-1)]\Big] \qquad \text{c-8}$$

$$= \frac{-1}{2i\pi(k-1)}\cdot 2i\sin[\pi(k-1)] \qquad \text{c-9}$$

I = 0 for all k ≠ 1 as (k-1) is always an integer and the sine of an integer times pi is zero.

KINETIC ENERGY

$$\langle p^2\rangle = \frac{1}{2a}\int_{-a}^{a} e^{i\pi(\alpha/2\pi+k)x/a}\,\frac{-d^2}{dx^2}\left[e^{-i\pi(\alpha/2\pi+1)x/a}\right]dx \tag{c-10}$$

$$= \frac{1}{2a}\left[\frac{\pi}{a}(\alpha/2\pi+k)\right]^2\int_{-a}^{a} e^{-i\pi(k-1)x/a}\,dx \tag{c-11}$$

$$= \left[\frac{\pi}{a}(\alpha/2\pi+k)\right]^2 \delta_{kl} \tag{c-12}$$

POTENTIAL ENERGY

$$\langle x^2\rangle = \frac{1}{2a}\int_{-a}^{a} x^2\, e^{-i\pi(\alpha/2\pi+k)x/a} \cdot e^{i\pi(\alpha/2\pi+1)x/a}\,dx \tag{c-13}$$

$$= \frac{1}{2a}\int_{-a}^{a} x^2 e^{-i\pi(k-1)x/a}\,dx \tag{c-14}$$

For k = 1

$$\langle x^2\rangle = \frac{1}{2a}\int_{-a}^{a} x^2\,dx = \frac{a^2}{3} \tag{c-15}$$

For k ≠ 1, integration by parts is used.

$$\langle x^2\rangle = \left[\frac{-x^2\, e^{-i\pi(k-1)x/a}}{i\pi(k-1)/a} - \frac{2x\, e^{-i\pi(k-1)x/a}}{[i\pi(k-1)/a]^2} - \frac{2\, e^{-i\pi(k-1)x/a}}{[i\pi(k-1)/a]^3}\right]_{-a}^{a} \tag{c-16}$$

$$\langle x^2 \rangle = \frac{-a^3}{i\pi(k-1)}\left[e^{-i\pi(k-1)} - e^{i\pi(k-1)}\right] - \frac{2a^3}{[i\pi(k-1)]^2} \cdot$$

$$\left[e^{-i\pi(k-1)} + e^{i\pi(k-1)}\right] - \frac{2a^3}{[i\pi(k-1)]^3}\left[e^{-i\pi(k-1)} -\right.$$

$$\left. e^{i\pi(k-1)}\right] \qquad \text{c-17}$$

Using c-6 and c-7 the exponentials can be simplified to:

$$e^{-i\pi(k-1)} - e^{i\pi(k-1)} = 2i \sin[(k-1)\pi] = 0$$

$$e^{-i\pi(k-1)} + e^{i\pi(k-1)} = 2 \cos[(k-1)\pi]$$

$$\langle x^2 \rangle = \frac{4a^3 \cos[(k-1)\pi]}{\pi^2 (k-1)^2} \qquad \text{c-18}$$

BIBLIOGRAPHY

1. G.G. Hall, R.D. Levine, J.Chem. Phys., 49, 51, (1968)
2. N.F. Mott, H.S. Massey, "Theory of Atomic Collisions", third edition, Oxford, 1965
3. J. von Neumann, "Mathematical Foundation of Quantum Mechanics", trans. from the German ed. by R. Beyer, Princeton U. Press, (1955)
4. A. Einstein, B. Podolsky, N. Rosen, Phys. Rev., 47, 777, (1935)
5. D. Bohm, Phys. Rev., 85, 166, (1952)
6. J.S. Bell, Rev. Mod. Phys., 38, 447, (1966)
7. J.M. Jauch, C. Piron, Helv. Phys. Acta 36, 827, (1963)
8. A.M. Gleason, J. Math. & Mech. 6, 885, (1957)
9. D. Bohm, J. Bub, Rev. Mod. Phys. 38, 453, (1966)
10. A. Siegel, N. Wiener, Phys. Rev. 101, 429, (1956)
11. J.H. Tutsch,Rev. Mod. Phys. 40, 232, (1968)
12. A. Daneri, A. Loinger, G.M. Prosperi, Nuc. Phys., 33, 297, (1962)
13. A.L. Licht, J. Math. Phys., 7, 1656, (1966)
14. D. Bohm, J.P. Vigier, Phys. Rev., 96, 208, (1954)
15. D. Kershaw, Phys.Rev. 136, B1850, (1964)
16. E. Nelson, Phys. Rev., 150, 1080, (1966)
17. L. De La Pena-Auerbach, J. Math. Phys., 10, 1620, (1969)
18. A. Messiah, "Quantum Mechanics", Wiley, third printing, (1965)
19. L. de Broglie, C.R. Acad. Sci. 264B, 1041, (1967)
20. L. de Broglie, C.R. Acad. Sci., 183, 447, (1926); 184, 273, (1927)
21. W. Pauli, "Collected Scientific Papers", vol. 2, p.608, Interstate Publishers, (1964)

23. T.D. Newton, E.P. Wigner, Rev. Mod. Phys., 21, 400, (1949)
24. A.S. Wightman, Rev. Mod. Phys., 34, 845, (1962)

25. J.M. Jauch, C. Piron, Helv.Phys. Acta, 40, 559, (1967)

26. E. Schrodinger, "Collected Papers on Wave Mechanics", trans. from the German, Blackie and Son Ltd. (1928), p.2

27. Ibid. p.3

28. Ibid. p.28

29. Ibid. p.29

30. B.L. Van der Waerden, "Sources of Quantum Mechanics", p.275, North Holland Pub. Co. (1967), p. 275

31. M. Jammer, "Conceptual Development of Quantum Mechanics", McGraw-Hill, (1966)

32. J. von Neumann, "Mathematical Foundation of Quantum Mechanics", trans. from the German by R. Beyer, Princeton U. Press, p. 137, (1955)

33. Ibid. p.132-137

34. H. Bremerman, "Distributions, Complex Variables, and Fourier Transforms", Addison-Wesley, (1965)

35. M.J. Lighthill, "Introduction to Fourier Analysis and Generalized Functions", Cambridge U. Press, (1958)

36. A. Papoulis, "The Fourier Integral and its Application", McGraw-Hill, (1962)

37. R. Flurry, "Molecular Orbital Theories of Bonding in Organic Molecules", M. Dekker, (1968)

38. H.A. Bethe, E.E. Salpeter, "Quantum Mechanics of One and Two Electron Atoms", Academic Press, (1957)

39. Geo. E. Forsythe, "Finite Difference Methods for Partial Differential Equations", Wiley, (1960)

40. R.R. Roy, B.P. Nigam, "Nuclear Physics: Theory and Experiment", Wiley, (1967)

41. B. Kuppers, Master's Thesis, University of Manitoba, (1969)

42. E. Nelson, "Dynamic Theories of Brownian Motion", Princeton U. Press, 1968